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LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
VOLUME II: SOURCE CHARACTERIZATION

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13. ABSTRACT (*Maximum 200 words*)

A mathematical model was generated to predict toxic chemicals released from an explosion involving a Titan II, Delta II, or Titan IV launch vehicle. The model was based on a variety of scientific and engineering input: the chemical description of interacting rocket propellants, data from previous accidents involving these or similar launch systems, an analysis of vehicle failure modes and propellant mixing characteristics, and thermochemical properties of reacting rocket propellants and their combustion products. Outputs of the model include the chemical composition and average molecular weight of the fireball cloud, the adiabatic flame temperature, the fireball size, and the total heat release. Input variables to the model include the time and altitude of abort, the mixing ratio for liquid propellants, amounts of unreacted liquid rocket propellants thermally decomposed, and the amount of air entrained into the fireball cloud. The mathematical model has been encoded into Fortran 77 for integration with the Rocket Exhaust Effluent Diffusion Model (REEDM) currently used at the Vandenberg Air Force Base (VAFB) Space Launch Complex.

14. SUBJECT TERMS
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PREFACE

This final report was prepared by Martin Marietta Astronautics, PO Box 179, Denver, Colorado 80201 in accordance with CDRL Data Item Number A004 of Attachment 1 to Contract F08635-92-C-0056 (Martin Marietta Proposal Number P91-60091-3) as authorized by Contract Award dated 92 Aug 10 for the Armstrong Laboratory, Tyndall Air Force Base, Florida 32403. Efforts documented in this report were performed between August 1992 and August 1994. Captain Floyd Wiseman was the AL/EQS-OL project officer.

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EXECUTIVE SUMMARY

A. OBJECTIVE

The objective of this study was to model chemical source emissions which result from on-pad or in-flight accidents involving the Titan II, Delta II, and Titan IV launch vehicle systems. Incorporation of input data such as propellant loading, time and altitude of abort, failure mode, and degree of air entrainment into these analytical models was also required. As companions to this effort, laboratory tests were required to verify the derived analytical model, and development of a Fortran 77 computer program, comprising the algorithms developed during this project, was also needed. Results of these two related efforts are documented in separate reports. Subsequent to this effort, the Fortran code will be integrated into atmospheric dispersion computer programs operating at the Western Test Range at Vandenberg Air Force Base (VAFB) and the Eastern Test Range at Cape Canaveral Air Force Station (CCAFS).

B. BACKGROUND

Launch vehicle accidents, such as the Titan 34 D-9 explosion at VAFB in April 1986, result in the formation of hot and thermally buoyant fireballs, release considerable amounts of thermal energy, and emit a variety of chemicals into the atmosphere. These chemicals consist primarily of combustion products from the reacted liquid and solid rocket propellants, propellant decomposition products, and vaporized propellants. Release of these materials into the atmosphere can produce airborne concentrations of toxic chemicals which exceed local and federal environmental health regulations.

Calculations of toxic hazard corridors (THCs) for launch vehicle accidents are required to support pre-launch risk assessment, in-flight disaster response support, and, in the case of a catastrophic accident, accident response and damage assessment. Studies conducted previously, such as Project Pyro tests completed in 1968, were useful in describing vehicle failure modes, fireball sizes, and heat releases from these types of accidents. Data from these tests, however, showed a high degree of variability and did not address the nature or amounts of released chemicals. Uncertainties in cloud composition and temperature have forced conservative estimates of THCs, which in turn have restricted launch operations. More reliable and defensible THC estimates are required to support launch operations and to protect public health.

C. SCOPE

This document presents the methodology and results of analytical modeling used to predict the size, temperature, and chemical composition for fireballs resulting from launch vehicle accidents. Section I provides an introduction to the technology. Section II discusses the compilation of background information used for model development. This includes information from technical reports, journal articles, accident data, launch vehicle configurations, and propellant loadings. Section III discusses rocket propellant chemistry and includes propellant combustion equations for liquid rocket propellants (Aerozine-50, nitrogen tetroxide, RP-1, and liquid oxygen), and solid rocket propellants (PBAN and PBHT). Section IV presents the failure modes and mixing analysis conducted for this project. This section includes a critical review and technical analysis of the Project Pyro test data, which resulted from the only large scale tests with liquid rocket propellants conducted to date. Section V presents the detailed thermochemical models prepared for the Titan II, Delta II, and Titan IV launch vehicles. Conclusions and recommendations are presented in Sections VI and VII, respectively. Detailed calculations and supporting data for this project are included in the Appendixes.

D. METHODOLOGY

The model used in the prediction of chemical source emissions was based on a variety of scientific and engineering input. This input included the chemical description of interacting rocket propellants, data from previous accidents involving these or similar launch systems, an analysis of the possible vehicle failure modes and mixing characteristics for liquid rocket propellants, and thermochemical properties of reacting rocket propellants and their expected combustion products. In addition to the theoretical work performed during this study, a series of laboratory tests involving the combustion of varying types and quantities of rocket propellants was conducted. The purpose of these tests was to evaluate the mixing and interaction of solid and liquid rocket propellants, and to apply the data to the estimation of toxic chemicals released during a launch vehicle accident. Results of this test activity are documented in Reference 1.

Outputs of the mathematical model included the chemical composition and average molecular weight of the fireball cloud, the adiabatic flame temperature, the fireball size (diameter and volume), and the total heat released. Input variables to this model included the time and altitude at abort, the mixing ratio for liquid rocket propellants (determined by failure mode), amounts of unreacted liquid rocket propellants thermally decomposed, and the amount of air entrained into the fireball cloud. Models for the three launch vehicles studied were encoded into Fortran 77 and the source code delivered to VAFB for integration into the Rocket Exhaust Effluent Diffusion Model (REEDM) computer program installed on the Cyber 865 computer at the launch facility. Descriptions of the Fortran 77 code utilizing the mathematical model are compiled in Reference 2.

E. TEST DESCRIPTION

Thermochemical data used to construct the models were verified by a variety of independent sources. Rocket component manufacturers (McDonnell Douglas Aircraft Company, Martin Marietta Astronautics, Hercules, and United Technologies Chemical Systems Division) provided computer calculations for equilibrium compositions of the various rocket propellant formulations. The JANAF thermochemical tables as well as the Gordon-McBride program for the calculation of complex chemical equilibrium compositions, rocket performance, incident and reflected shocks, and Chapman-Jouguet detonations provided thermochemical reference data for most of the rocket propellants, combustion products, and thermal decomposition products investigated in this project. Thermochemical data for other chemicals not available in these sources were obtained from reputable literature sources or estimated using numerical techniques. Thermochemical and chemical equilibrium calculations predicted by the model were independently verified using a microcomputer program developed by Outokumpu Research. Degree of mixing calculations for propellant fireballs were generated using radiant heat flux analyses of 25,000 pound test for liquid oxygen/RP-1 and 1,000 pound test for Aerozine-50/nitrogen tetroxide reported by Project Pyro. Fireball size calculations were made using a model developed by the Marshall Space Flight Center. Solid propellant combustion characteristics were derived from fragmentation analysis provided by the Research Triangle Institute.

F. RESULTS

Source models were developed for the Titan II, Delta II, and Titan IV launch vehicles, as well as for solid propellant motor segments. The latter model was generated to predict chemical source emissions from ground handling accidents during stacking or destacking operations of the Delta II and Titan IV solid rocket motors.

The degree of liquid propellant mixing during an explosive event was estimated at 23 percent for Aerozine-50/nitrogen tetroxide propellant systems and 44 percent for RP-1/liquid oxygen systems. These percentages determined residual amounts of unreacted propellants which may be released into the fireball cloud. The selection of these values was made upon analysis of Project

Pyro heat flux data, which were variable and incomplete. Limitations on available heat flux data on Aerozine-50/nitrogen tetroxide propellants from the Project Pyro tests, for example, have resulted in uncertainties in the prediction of released liquid rocket propellants during an accident.

For vehicles employing both liquid and solid rocket propellants, the source models contained algorithms for the generation of two fireball clouds: an upper cloud consisting of liquid rocket propellants and their reaction products; and a lower cloud consisting of solid propellant reaction products. The use of two clouds in modeling these accidents results in two point sources from which atmospheric dispersion processes can begin. This approach is consistent with previous efforts in launch vehicle abort modeling, and is supported by photographic test data from previous launch vehicle accidents.

Although review of Project Pyro data suggests that air entrainment into the liquids cloud is negligible, considerable uncertainty exists with respect to this process. Air entrainment into fireball clouds can have a profound effect on the temperature and chemical composition of the clouds, and is driven by both physical (gas dilution and heat absorption) processes and chemical (afterburning with air) processes. Combustion reactions with atmospheric oxygen can reduce concentrations of toxic chemicals, such as hydrazine and unsymmetrical dimethylhydrazine, by converting them to more innocuous compounds, such as nitrogen, water vapor, and carbon dioxide. Because of the importance of air entrainment into launch vehicle abort modeling, a provision has been made for the incorporation of varying amounts of entrained air into each of the liquid cloud source models, with a suggested default value of zero air entrainment.

G. CONCLUSIONS

Source characterizations were performed for the Titan II, Delta II, and Titan IV launch vehicle systems and provided improvements over previous models in the understanding and application of propellant behaviors in a catastrophic accident. Results of these models correlated well with available technical information, such as large scale test results conducted by Project Pyro, laboratory test results conducted during this project, and post-accident investigations such as the Titan 34D-9 accident in 1986. The algorithms used to generate these models were encoded into Fortran 77 programming language and were tested on the Cyber computer at VAFB.

H. RECOMMENDATIONS

As with any analytical model, appropriate testing should be conducted to validate the results. Tests involving the explosive mixing of large quantities of liquid and solid rocket propellants should be performed, and results analyzed to provide improvements in the degree of propellant mixing and the amount of air entrained during an abort. Airborne concentrations and ground level depositions of released chemicals from these large-scale tests should be measured to validate both the source model and the dispersion programs used at the launch sites. The design and execution of such tests are critical, to ensure that measurements and their statistical uncertainties are obtained in an optimum and reliable manner. A provision for incorporation of radiant heat flux equations into the source models would also provide an improvement in the temperature-time profile of the fireball cloud and refine the existing models. Finally, because the Fortran 77 program developed during this program was an engineering prototype, more rigorous testing and evaluation are required to upgrade the computer program for operational use.

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SECTION I

INTRODUCTION

A. OBJECTIVE

Military spacecraft launches at the Eastern and Western Test Ranges require pre-launch risk analyses, in-flight disaster response support, and, in the case of a catastrophic accident, abort damage assessment. Calculation of toxic hazard corridors (THCs) is an important element of each of these requirements. Reductions in allowable public exposure to toxic vapors released in launch accidents threaten to impose constraints on launch operations as THCs may reach civilian populations more frequently than in the past.

Current atmospheric dispersion models used for establishing launch support THCs depend on accurate estimates of toxic vapor source strength to produce accurate "footprints" of downwind vapor concentration. Uncertainties in source cloud composition for various accident scenarios, especially those involving fire, explosion, and vehicle destruction, force conservative assumptions that may extend THCs and unnecessarily restrict launch opportunities. This makes development of accurate, defensible estimates of source cloud characteristics imperative for launch safety planning and emergency response.

This effort was designed to characterize the chemical and thermal effects of launch vehicle explosions involving a Titan II, Delta II, or Titan IV missile, and solid rocket motors or motor segments from these missiles. The purpose of this effort was to develop a mathematical model to predict fireball parameters, such as total heat released, chemical composition, adiabatic flame temperature, fireball shape and size, and air entrained from accident input parameters, such as failure mode and abort altitude. The determination of these fireball parameters could then be integrated into an existing atmospheric dispersion computer program in use at Vandenberg Air Force Base (Reference 3).

B. BACKGROUND

In 1982, the Air Force, along with other agencies, investigated the expected toxic chemical source strengths and downwind compositions arising from an accident involving the Titan II Operational Weapons System. That study investigated chemical interactions and atmospheric dispersion processes during an accident in which liquid nitrogen tetroxide mixed with liquid Aerozine-50, resulting in a hypergolic explosion. Data obtained during the study included fireball temperatures and heat fluxes, fireball diameters, gas product compositions, gas densities, and tabulations of thermochemical properties for hypergolic propellants and reaction products.

In 1983, a comprehensive study was funded by the Air Force to obtain, evaluate, and compile all pertinent existing data on hazards to satellite and operational launch vehicles resulting from solid and liquid propulsion systems. Results of this study were incorporated into a systems users manual entitled Space Propulsion Hazards Analysis Manual (SPHAM), and included documentation on numerous vehicle types and propellant combinations.

As a result of an in-flight explosion of a Titan 34D vehicle from the Vandenberg Launch Complex in April 1986, another study was funded by the Air Force to determine toxic chemical emissions from this vehicle. This study was unique, in that the contribution of combustion products of the solid rocket booster to the thermal and chemical environment of the resultant fireball was determined.

On August 10, 1992, Martin Marietta was awarded an Air Force contract to model combustion clouds resulting from an accident or range safety destruction involving a Titan II, Delta II, or Titan IV launch vehicle. As part of this contract, a more detailed investigation of credible failure modes and propellant mixing for these vehicles was required. Laboratory testing and software development were also authorized as part of this study.

C. SCOPE

The purpose of this project was to characterize the chemical composition, size, shape, and thermal properties of toxic vapor clouds resulting from accidents involving launch vehicles powered by solid and liquid rocket propellants. This effort involved collecting vehicle configurations, propellant loadings, and failure mode information on a number of United States Air Force (USAF) launch vehicles, and modeling the accident results. Algorithms were developed to provide toxic vapor cloud source strength estimates. These algorithms formed the basis for the Fortran 77 code intended as input to the REEDM code installed at VAFB.

Launch vehicles studied in this project include the Titan II, Delta II, Titan IV, Delta II Solid Rocket Motors Segments, and Titan IV Solid Rocket Motors Segments. To account for possible hazards during an in-flight accident, the fireball properties were evaluated for accidents between the launch pad and 10,000 feet. Fireball properties were characterized up to the point when the generation of chemical energy within the fireball ceases (burnout), and the effort was limited to each vehicle's primary propellants. The contribution of secondary propellants, such as upper stage propellants, was not considered in this effort.

This program was comprised of several key work packages, as described in the following paragraphs.

1. Compilation of Background Information

Background technical information and empirical relationships used to generate a mathematical model of chemical source emissions were provided by a thorough review of past literature, available test data, research and development reports, and accident investigations.

2. Failure Modes and Mixing Analysis

Because the release of toxic chemicals in an launch vehicle accident is dependent on the degree in which liquid rocket propellants mix and react, a determination of the failure modes and the mixing characteristics of propellants was required. To complete this analysis, a review of test data involving reacting rocket propellants, in particular data from Project Pyro tests (Reference 4), was conducted. These data proved to be most useful, especially in modeling the amount of heat evolved and the quantity of residual propellants released. This review and its subsequent engineering analysis served as the basis for the development of the failure modes and mixing analysis for launch vehicle accidents.

3. Thermochemical Analysis

The characterization of chemical composition, fireball size, and heat evolution from a launch vehicle accident was determined using a variety of empirical and theoretical equations developed in previous studies (References 5,6). Emphasis was placed on improved descriptions of propellant decomposition processes and on incorporation of entrained air. Enhancements made to the mathematical model in these two areas have greatly improved predictions of toxic chemical releases.

4. Laboratory Testing

Laboratory testing was performed to evaluate the formation of toxic chemicals under a variety of propellant combustion conditions, and to compare these results with predicted values. Results which were inconsistent with chemical theory were used to modify the model when appropriate. Test philosophy, methods, and results were compiled in a separate report (Reference 1) and are included in this report only to the degree that their discussion contributes to the developed source model.

5. Software Development

Engineering prototype software was developed from the mathematical model. The purpose of the software was to provide the chemical source data to the REEDM dispersion code for subsequent calculations not within the scope of this effort. The software code was developed on an IBM PC/DOS machine using Fortran 77 programming language, and was fully tested for six launch vehicle abort test cases. In addition, the code was developed in a modular format for easy expansion with new input data or incorporation of new vehicles. Documentation, including the source code listing, users' manual, flowcharts, logic diagrams, and variable definitions are included in Reference 2. The results of this work package are presented in this report only to the extent needed to clarify the mathematical model for chemical source emissions.

SECTION II

COMPILATION OF BACKGROUND INFORMATION

Information on the characterization of launch vehicle explosions was obtained from a variety of sources. Journal articles, government reports, and accident data obtained for the 1988 study (Reference 6) were reviewed for applicability to the present study. A library search was also initiated to identify pertinent documents specific to the launch vehicles and propellant systems modeled during this effort. Computer-aided library searches were used to find primary technical reports and literature. Searches were conducted in two technical databases: National Technical Information Service (NTIS) 1985 to 1992, and the Applied Science and Technology (AST) database 1983-1992.

Stage configurations and nominal propellant loadings were obtained for the Titan II, Delta II, and Titan IV launch vehicles. Delta II loadings have been obtained with the assistance of D. Dargitz of the Missile Flight Control Branch, Vandenberg Air Force Base and R. Nyman of Acta, Inc. Titan II and Titan IV loadings have been obtained from internal Martin Marietta sources. Solid rocket propellant information was obtained by the manufacturers, United Technologies Chemical Systems Division (Titan IV Solid Rocket Motor) and Hercules (Delta II Graphite Epoxy Motor). Information obtained from these sources were used to determine nominal combustion conditions for these vehicles, and to provide a foundation for the mathematical development of the chemical source algorithm.

References related to past accidents and credible failure modes for these launch vehicles have been obtained and reviewed for applicability to the present study. This review has included data on the fragmentation of solid rocket motor segments (Titan IV and Delta II) during an in-flight abort.

Several references have been identified with respect to the chemistry of interacting rocket propellants. Particular emphasis has been made on the combustion of unsymmetrical dimethylhydrazine (UDMH) in air, the reaction of nitrogen tetroxide with atmospheric water vapor to form a nitric acid azeotrope, and chamber wall reactions with Aerozine-50, which were pertinent to the test program. Intrinsic to this review was the thermal decomposition processes for the liquid rocket propellants: Aerozine-50, RP-1, and nitrogen tetroxide. A series of references was obtained in which decomposition temperatures and resultant decomposition products were reported.

Thermochemical properties of chemical reactants (liquid and solid rocket propellants) and chemical products (combustion products, reaction products with air, thermal decomposition products, and vaporized propellants) were obtained from thermochemical tables, chemical reference books, rocket exhaust equilibria programs, and other published sources. Equilibrium compositions of combustion products from stoichiometric burning of liquid and solid rocket propellants were determined using rocket exhaust equilibria computer programs.

A compilation of applicable documents related to this effort is included in the Bibliography, and specific references to these documents in this report is maintained in the Reference Section.

SECTION III

ROCKET PROPELLANT CHEMISTRY

Combustion properties of liquid and solid rocket propellants used on the Titan II, Delta II, and Titan IV launch vehicles were evaluated using a variety of sources. Properties of interest to this study were the identification of combustion products, adiabatic flame temperatures, the chemical composition of the reacting propellants, the thermal stability of unreacted propellants, and reactions of unreacted propellants or their combustion products with entrained air. In addition, reactions between solid and liquid propellants were considered, as well as gas-phase interactions between combustion products and unreacted vaporized propellants.

Propellants studied were Aerozine-50 (A-50), a blended liquid amine fuel, nitrogen tetroxide (N_2O_4), a volatile, reddish brown liquid oxidizer, RP-1 a kerosene-based hydrocarbon fuel, liquid oxygen (LOX) the cryogenic oxidant source, UTP-3001B, the United Technologies formulation for the Titan IV solid rocket motor (SRM), and QDL, the Hercules formulation for the Delta II Graphite Epoxy Motor (GEM). The solid propellants consist of an organic binder, metallized aluminum powder, ammonium perchlorate solid oxidizer, and small amounts of burn rate catalysts. The Aerozine-50 liquid rocket fuel is a 50/50 mixture, by weight, consisting of hydrazine (N_2H_4) and unsymmetrical dimethylhydrazine ($C_2H_8N_2$, or UDMH).

A. AEROZINE-50/NITROGEN TETROXIDE

1. Bipropellant Combustion

The stoichiometric chemical reaction between Aerozine-50 fuel and nitrogen tetroxide oxidizer can be most simply represented by Equation (1)

$$\frac{2}{3} N_2H_4 + \frac{1}{3} C_2H_8N_2 + N_2O_4 \rightarrow \frac{8}{3} H_2O + 2N_2 + \frac{2}{3} CO_2 \tag{1}$$

The heat of reaction for this ideal combustion of Aerozine-50 with nitrogen tetroxide is -224.3 kilocalories (-2.243×10^5 calories) per gram mole N_2O_4 reacted. If the entire amount of evolved heat is used to heat the combustion products to a final equilibrium temperature (i.e., no heat loss to the surrounding environment), this temperature, termed the adiabatic flame temperature, would be 4135 K. This temperature is sufficiently high to decompose the reaction products to form unstable chemical products. In practice, complex chemical equilibrium programs are used to perform iterative calculations in which the product composition is varied, and the Gibbs Free Energy (GFE) of the reaction is calculated. A final solution of product composition is determined when the GFE is minimized over the determined reactant (propellant) and product (combustion gases) compositions. These computer programs predict the thermodynamically stable products for propellant reactants under adiabatic conditions, and are used widely by propulsion engineers for rocket performance calculations. Combustion of Aerozine-50 with nitrogen tetroxide calculated by standard rocket exhaust equilibrium programs also results in carbon monoxide, molecular hydrogen, atomic hydrogen, nitric oxide, atomic oxygen, and hydroxide radical in accordance with Equation (2).

$$\begin{aligned} &0.6522\ N_2H_4 + 0.3478\ C_2H_8N_2 + 1.0217\ N_2O_4 \rightarrow \\ &2.0866\ H_2O + 1.9823\ N_2 + 0.3149\ CO_2 + 0.3808\ CO \\ &+ 0.3582\ H_2 + 0.1784\ H + 0.0761\ NO + 0.1017\ O \\ &+ 0.2406\ O_2 + 0.3243\ OH \end{aligned} \tag{2}$$

The calculated heat of reaction using the rocket exhaust equilibrium program is -1.475 x 10^5 calories per gram mole reacted, and the adiabatic flame temperature is 2918 K. The negative sign on the heat term indicates a heat release. This heat release was calculated using the standard heats of formation of chemical reactants and gaseous reaction products for the stoichiometric hypergolic reaction and will be discussed in more detail in Section V. The large drop in heat release from the simple reaction depicted in Equation (1) to the reaction computed using Gibbs Free Energy minimization techniques in Equation (2) is due to the formation of high energy products such as atomic oxygen, atomic hydrogen, and hydroxide radical.

As a result of a launch vehicle accident, the high thermal energy imparted by the combustion of the liquid rocket propellants is expected to form high energy reactive intermediates as represented in Equation (2). As the vapor cloud is stabilized, allowed to cool, and dispersed by prevailing winds, these reactive intermediates will recombine to form more thermally stable species with the concurrent release of additional heat. Thus the actual gas composition of the fireball cloud will change based upon its instantaneous fireball temperature. The "true" fireball composition therefore is expected to be a trade-off between the idealized combustion represented in Equation (1) and the high-energy composition represented in Equation (2). This process is actually temporally driven in that the initial explosive event produces high internal thermal energy with little thermal interchange with the environment, resulting in high energy chemical products. As thermal interchange with the environment becomes more significant (air entrainment and subsequent dispersion), the more thermally stable chemicals are formed. The formation of thermally stable chemicals from reactive intermediates becomes complete when the entire thermal energy of the fireball cloud has been absorbed and dissipated by the environment.

The selection of equilibrium composition for launch vehicle modeling purposes is complicated by this shifting equilibrium consideration, and will be discussed in more detail in Section V.

Thermal and physical properties for the Aerozine-50/nitrogen tetroxide bipropellant system are compiled in Table 1.

2. Chemical Intermediates Identified in the A-50/Nitrogen Tetroxide Reaction

In addition to the products identified in Equation (2), several competing side reactions occur upon mixing of the two hypergolic liquid propellants. Over 50 chemical species have been isolated and identified either as chemical intermediates or condensed phase reaction products in the A-50/N_2O_4 reaction.

Some of these side products (such as hydrazine nitrate and hydrogen azide) have been identified as the reaction condensates responsible for the "hard start" and "popping" phenomena characteristic of hydrazine-N_2O_4 pulsed rocket engines (Reference 7). While these particular chemical residues affect engine performance and ignition threshold, the instability of these compounds at elevated temperatures make their survivability in a hot hypergolic fireball improbable. Other chemical reaction products are more stable, especially at lower temperatures (500 K) and the presence of these compounds in a fireball may significantly impact the toxicity of the resultant cloud. The chemical species in this category include dimethylnitrosamine (NDMA), methyl amine, dimethyl amine, formaldehyde, hydrogen cyanide, ammonia, and formaldehyde dimethylhydrazone (FDH). In addition to these reaction products, unreacted propellant vapors (hydrazine vapor, UDMH vapor, nitrogen dioxide) resulting from incomplete combustion and volatilization of excess propellant will also pose a health hazard upon atmospheric dispersion, since both the hydrazine fuel and nitrogen tetroxide oxidizer are extremely toxic, in both the liquid and vapor phases.

TABLE 1. LIQUID PROPELLANT SOURCE DATA, AEROZINE-50/NITROGEN TETROXIDE BIPROPELLANT SYSTEM.

Propellant Type:	FUEL:	Aerozine-50	OXIDIZER:	Nitrogen Tetroxide
Usage:		Titan II (Stage I, II); Titan IV (Stage I, II)		

PHYSICAL PROPERTIES

Density (25°C):	0.8987 g/cm^3	1.433 g/cm^3 (liquid)
Chemical Formula:	$C_{0.6956}H_{5.3911}N_2$	N_2O_4
Molecular Weight:	41.805 g/mole	92.016 g/mole
Vapor Pressure (Liquid), 298K	138.4 mm Hg	898.6 mm Hg

THERMAL PROPERTIES

Heat of Formation, 298 K:	+12.310 kcal/mole @298K *	-4.676 kcal/mole @ 298.15K, 0.1 MPa
Heat of Vaporization at T:	+8.048 kcal/mole @ NBP = 343K	6.790 kcal/mole, 298K
Heat of Combustion:	-312.112 kcal/mole (298 K)	
Heat Capacity, Liquid:	0.732 cal/g-K (298 K)	0.378 cal/g-K,298 K,0.1 MPa NO_2(g):8.87cal/mole/K, STP

*Includes Heat of Mixing (ΔH_{mix} = 0.257 kcal/mole)

THERMODYNAMIC PROPERTIES OF COMBUSTION PRODUCTS

Component	Chamber	Exit Equil	Component	Chamber	Exit Equil
CO_2		5.21%	NO		1.26%
CO		6.30%	O		1.68%
H_2O		34.52%	O_2		3.98%
H_2		5.93%	OH		5.37%
N_2		32.80%			
H		2.95%			

Adiabatic Flame Temperature 2918 K

Figures 1 and 2 show two postulated reaction pathways for the formation of these side products (Reference 8). Few of these secondary reaction products are predicted by chemical equilibrium considerations; most products identified in a reaction mixture are frozen in a non-equilibrium state due to kinetic barriers. Since activation energies for the various reaction pathways are not readily available, prediction of the amounts of these secondary products in a given hypergolic reaction is difficult.

3. Hydrazine Decomposition

High temperatures present in a fireball can initiate decomposition of excess propellants. Partial decomposition, Equation (3) of hydrazine can yield ammonia and nitrogen, while complete decomposition as represented in Equation (4) yields nitrogen and hydrogen as major products. The combination of these two decomposition reactions results in an overall expression for the decomposition of hydrazine in Equation (5).

$$3\ N_2H_{4\,(g)} \rightarrow 4\ NH_3 + N_2 \qquad \text{Partial Decomposition} \qquad (3)$$

$$N_2H_{4\,(g)} \rightarrow N_2 + 2\ H_2 \qquad \text{Complete Decomposition} \qquad (4)$$

$$N_2H_4\ (g) \rightarrow NH_3 + \frac{1}{2}\ N_2 + \frac{1}{2}\ H_2 \qquad \text{Overall Decomposition} \qquad (5)$$

Hydrazine decomposition occurs in the vapor phase between 100°C and 200°C, and the calculated adiabatic flame temperature for the overall decomposition reaction is 1895 K with the heat of reaction of -3.373×10^4 calories.

4. Hydrazine Oxidation

In a hot gaseous fireball, entrained air has a significant role in the removal of hydrazine. The autoignition temperature of hydrazine in the presence of air is reported to be 270° C (Reference 9). The high-temperature oxidation reaction of hydrazine with molecular oxygen is described in Equation (6).

$$N_2H_{4\,(g)} + O_2 \rightarrow N_2 + 2\ H_2O \qquad (6)$$

In addition to the main reaction which produces nitrogen and water vapor, there are side reactions which produce ammonia and are largely heterogeneous in nature. The rates of the main reactions, as well as the side reaction in which ammonia is produced, are strong functions of surface area and geometric factors. The oxidation reaction represented in Equation (6) releases 1.38×10^5 calories per gram mole hydrazine oxidized. A distinction is made between the high-temperature air oxidation of hydrazine (as would be expected during fireball formation and growth) and low-temperature air oxidation (as would be expected during the cooling of the fireball cloud upon dispersion). The latter case is especially interesting because the homogeneous oxidation reaction of hydrazine at ambient temperatures is expected to be very slow or negligible. The atmospheric interactions of fireball constituents after cooling are discussed in Section III E.

5. Hydrazine Vaporization

Excess hydrazine not thermally decomposed or reacted with atmospheric oxygen may be present in the fireball cloud as free vapor. The reaction equation and heat required to vaporize one gram mole of liquid hydrazine is:

$$N_2H_4\ (l) \rightarrow N_2H_4\ (g) \qquad \Delta H_{vap,298} = +10380 \text{ calories/mole} \tag{7}$$

6. UDMH Decomposition

Spontaneous ignition of UDMH in the absence of oxygen occurs at a partial pressure of 5.7 mm Hg and at 514°C (Reference 10). Thermal decomposition of UDMH is more complex than that of hydrazine, the UDMH reaction beginning at 300°C and being complete at 800°C (Reference 11). In addition, the presence of hydrazine accelerates the rate of UDMH decomposition. The decomposition products includes methane and nitrogen, plus smaller amounts of hydrogen, ethane, ammonia, and hydrogen cyanide. The main decomposition reaction, represented in Equation (8), releases 5.594×10^4 calories per gram mole UDMH, and has an adiabatic flame temperature of 1685 K.

$$C_2H_8N_{2\ (g)} \rightarrow 2\ CH_4 + N_2 \tag{8}$$

7. UDMH Oxidation

High-temperature oxidation of UDMH produces carbon dioxide, water vapor, and nitrogen in accordance with Equation (9). This reaction is very exothermic and releases 4.39×10^5 calories per mole UDMH oxidized. The minimum pressure required for ignition occurs near UDMH + $2O_2$ (Reference 10). Nitrogen, carbon monoxide and water vapor are produced, along with hydrogen, methane and ammonia in smaller amounts. Weak ignition occurs in very rich (4UDMH + $1O_2$) mixtures, and reaction products are similar to those observed under thermal decomposition conditions.

$$C_2H_8N_2(g) + 4O_2 \rightarrow 2CO_2 + 4\ H_2O + N_2 \tag{9}$$

Formaldehyde dimethylhydrazine (FDH) is also formed, as well as diazomethane, dimethylamine, ammonia, and nitrosodimethylamine (NDMA) in reactions between UDMH and air. The reaction stoichiometry for the production of FDH is presented in Equation (10).

$$3\ C_2H_8N_2(g) + 2O_2 \rightarrow 2\ (CH_3)_2NNCH_2 + 4\ H_2O + N_2 \tag{10}$$

8. UDMH vaporization

Excess unreacted UDMH liquid may absorb heat from the fireball and become vaporized in accordance with Equation (11)

$$C_2H_8N_2\ (l) \rightarrow C_2H_8N_2\ (g) \qquad \Delta H_{vap,298} = +8366 \text{ calories/mole} \tag{11}$$

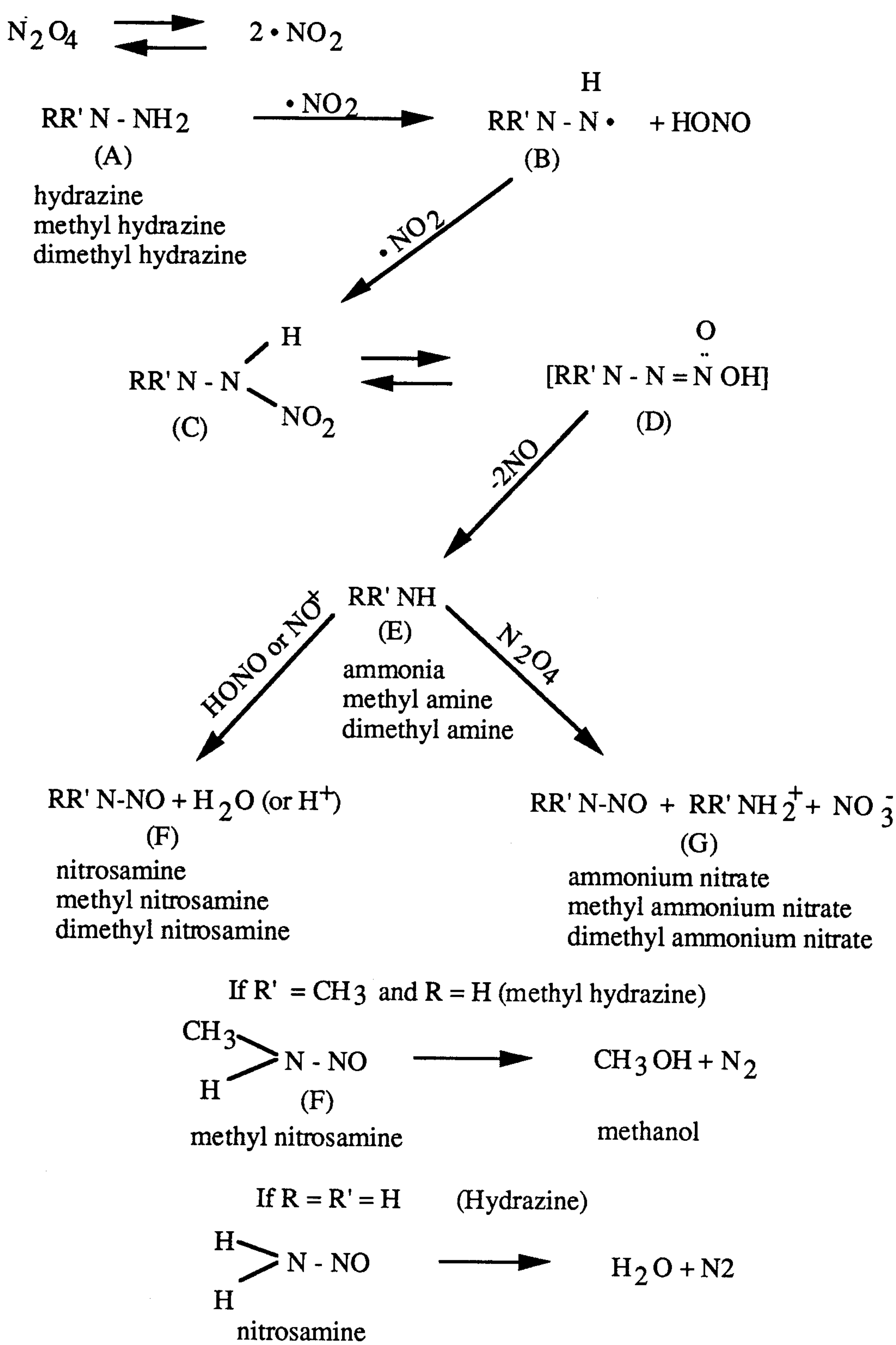

Figure 1. Proposed Free Radical Mechanism For Reaction Of N_2O_4 With Hydrazines.

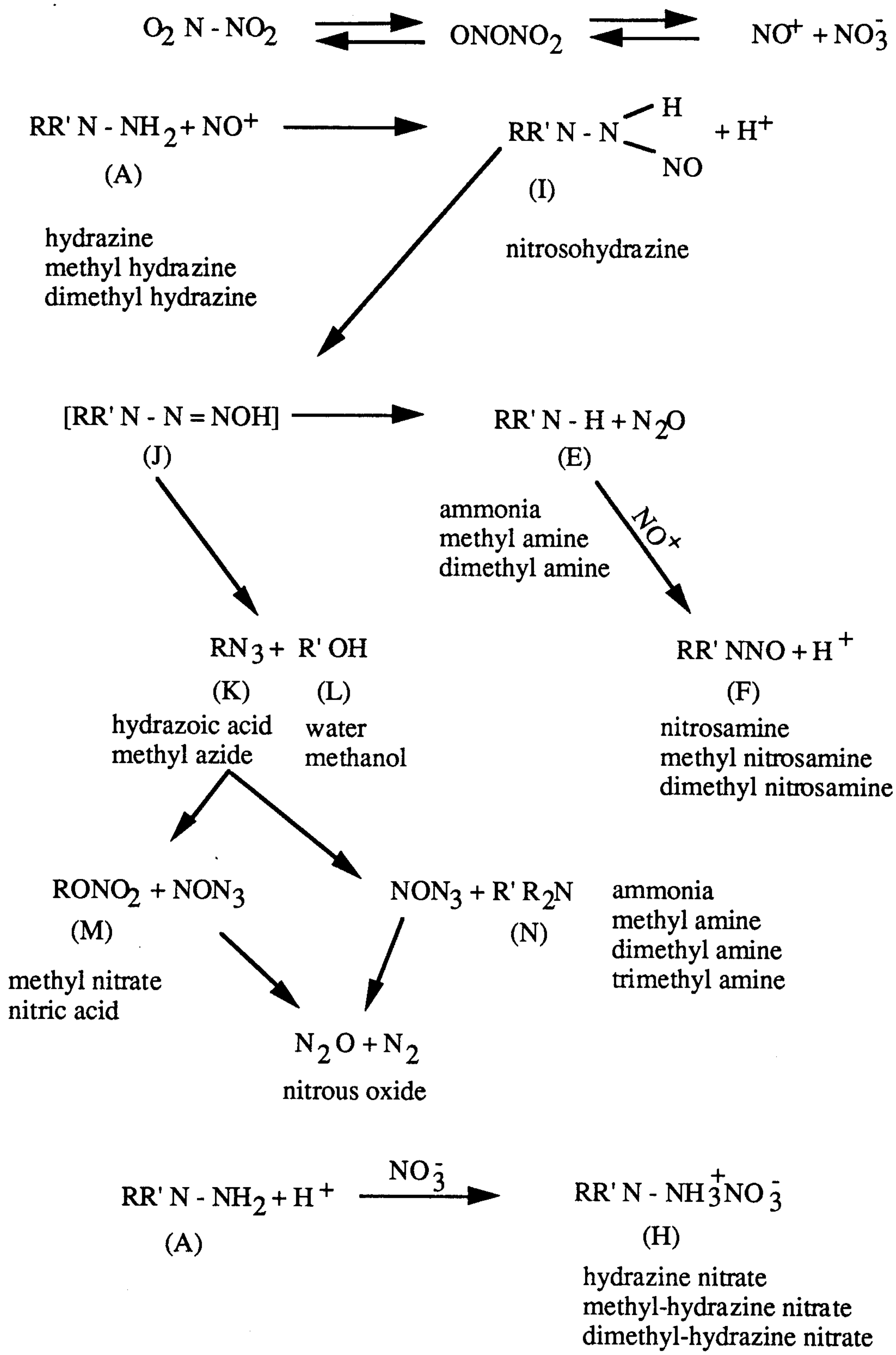

Figure 2. Proposed Nitrosation Mechanism For Reaction Of N_2O_4 With Hydrazines.

9. Nitrogen Tetroxide Chemistry

Nitrogen tetroxide liquid is converted to nitrogen tetroxide vapor by the application of thermal energy:

$$N_2O_4\ (l) \xrightarrow{heat} N_2O_4\ (g) \qquad \Delta H_{vap,\ 298} = +\ 6790\ \text{cal/mole} \tag{12}$$

Nitrogen tetroxide also exists in equilibrium with nitrogen dioxide:

$$2\ NO_2\ (g) \rightleftarrows N_2O_4\ (g) \qquad \Delta H_{298} = -13600\ \text{cal/mole}\ N_2O_4 \tag{13}$$

The proportion of nitrogen tetroxide and nitrogen dioxide in the vapor phase is temperature-dependent. At temperatures above 100°C (373 K), unreacted nitrogen tetroxide gas is essentially dissociated into nitrogen dioxide. The ratio of nitrogen tetroxide to nitrogen dioxide is controlled by the equilibrium constant for the association reaction:

$$Kp = \frac{pN2O4}{(pNO2)^{2}} \tag{14}$$

Where pN_2O_4 = partial pressure N_2O_4 vapor at equilibrium
pNO_2 = partial pressure NO_2 vapor at equilibrium

The equilibrium constant K_p for the association of two molecules of nitrogen dioxide gas into one molecule of nitrogen tetroxide gas may be calculated using the Gibbs free energy function:

$$\Delta G^\circ = -RT \ln K_p = -13600 + 41.6T \tag{15}$$

where R = gas constant (1.9872 calories/mole-K)
K_p = association equilibrium constant (atm^{-1})
T = Temperature (K)
ΔG° = Gibbs free energy (calories/mole)

The equilibrium mole fractions of nitrogen tetroxide gas and nitrogen dioxide gas as a function of temperature are presented in Table 1. In this case, the mole fraction of nitrogen oxide vapors (NO_2 or N_2O_4) are equal to the partial pressures of the vapors at one atmosphere total pressure. The percent dissociation of nitrogen tetroxide into nitrogen dioxide is also presented in Table 2.

$$\text{Percent Dissociation} = \frac{pNO2 \times 100}{pNO2 + 2pN2O4} \tag{16}$$

TABLE 2. EQUILIBRIUM COMPOSITION OF NITROGEN TETROXIDE AND NITROGEN DIOXIDE IN THE VAPOR PHASE AS A FUNCTION OF ABSOLUTE TEMPERATURE.

(P_{Total} = 1 atmosphere)

Temperature, K	Mole Fraction N_2O_4	Mole Fraction NO_2	Percent Dissociation
298	0.698	0.302	18
313	0.539	0.461	30
323	0.426	0.574	40
373	0.066	0.934	88

Nitrogen dioxide, may undergo thermal decomposition to nitric oxide and molecular oxygen as represented in Equation (17). This is a reversible reaction, and the relative amounts of nitrogen dioxide and nitric oxide (NO) depends on the equilibrium temperature. Dissociation of nitrogen dioxide begins at 150°C (423 K), and at 600°C (873 K) conversion to nitric oxide is complete. Upon cooling to room temperature, the NO reacts with available oxygen to form the reddish-brown colored NO_2. Nitrogen dioxide is the thermodynamically favored species at room temperature (25°C or 298 K), as evidenced by the positive sign on the Gibbs free energy function at this temperature. Equilibrium compositions of nitrogen dioxide, nitric oxide, and molecular oxygen as a function of absolute temperature are presented in Figure 3.

$$NO_2\,(g) \rightleftarrows NO\,(g) + \frac{1}{2}\,O_2\,(g) \quad \Delta G_{298} = +8930 \text{ cal/mole} \tag{17}$$

Nitric oxide may undergo subsequent thermal decomposition to molecular nitrogen and molecular oxygen as indicated in Equation (18). In this example, the Gibbs free energy function is negative at 298 K, indicating this reaction is thermodynamically favored at room temperature. Equilibrium compositions of nitric oxide, nitrogen, and oxygen as a function of absolute temperature are presented in Figure 4.

$$NO(g) \rightleftarrows \frac{1}{2}N_2\,(g) + \frac{1}{2}O_2(g) \qquad \Delta G_{298} = -20500 \text{ cal/mole} \tag{18}$$

From a thermodynamic standpoint, the dissociation of nitric oxide to molecular nitrogen and molecular oxygen is favored up to about 3000°C (3273 K). Only at temperatures above 3000°C can NO form from its respective elements. At 2273 K, 1.2 volume percent of nitric oxide is in equilibrium with molecular nitrogen and molecular oxygen. At 3273 K, this value is increased to 5.3 volume percent. The nitric oxide thus formed must be rapidly quenched below 1000°C in order to prevent the reformation of nitrogen and oxygen.

Of particular significance in this discussion is the observation that the dissociation of nitric oxide to nitrogen and oxygen, although thermodynamically favored at room temperature, is extremely difficult to achieve thermally or in the presence of catalysts. The study of the catalytic decomposition of nitric oxide has been widely investigated, especially for automobile emissions. The noble metals, platinum and iridium, catalyze the decompositions of nitric oxide at temperatures as low as 670°C (943 K) (Reference 12). The decomposition of nitric oxide is a second-order reaction, comprised of two components: a homogeneous reaction that dominates at high temperatures (above 876 K), and a heterogeneous wall catalyzed reaction that controls at lower temperatures (below 876 K). Activation energies for the homogeneous and heterogeneous reactions are 82 kilocalories per mole and 21.4 kilocalories per mole, respectively.

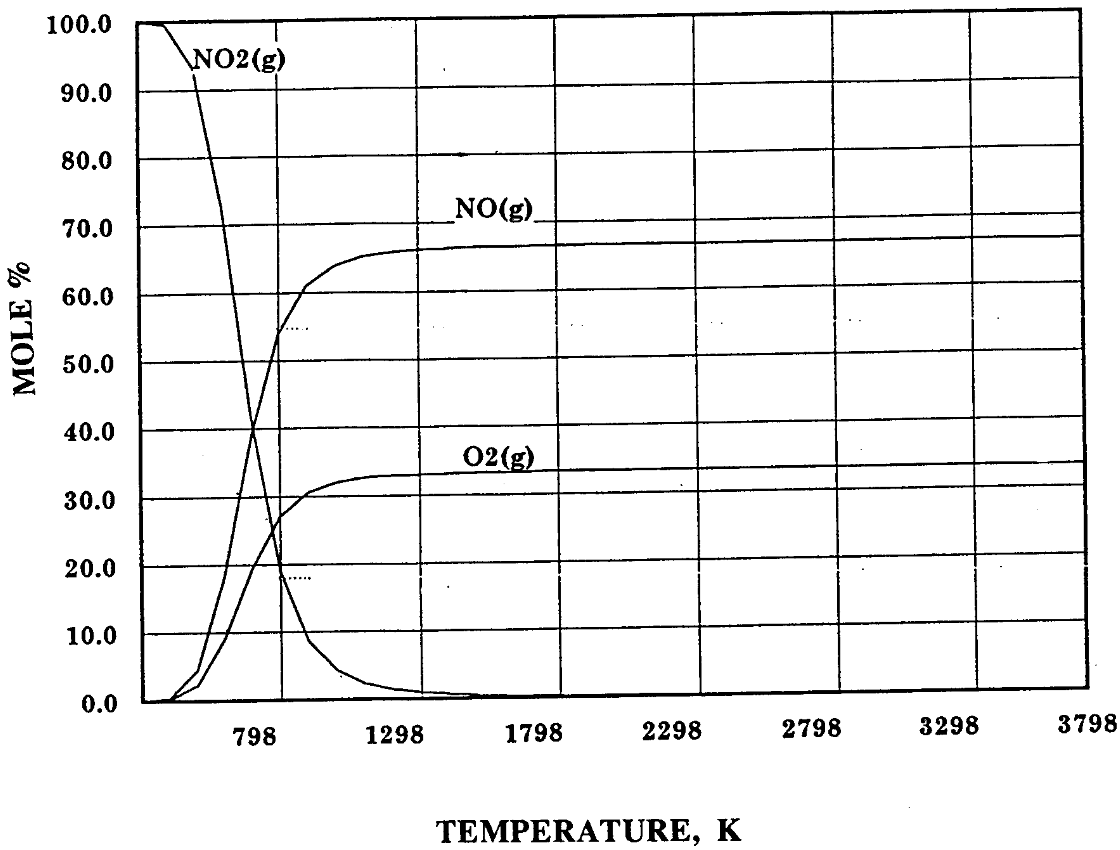

Figure 3. Equilibria Involving Nitrogen Dioxide, Nitric Oxide, And Oxygen.

$$NO_2\ (g) \rightleftarrows NO\ (g) + \frac{1}{2}\ O_2\ (g)$$

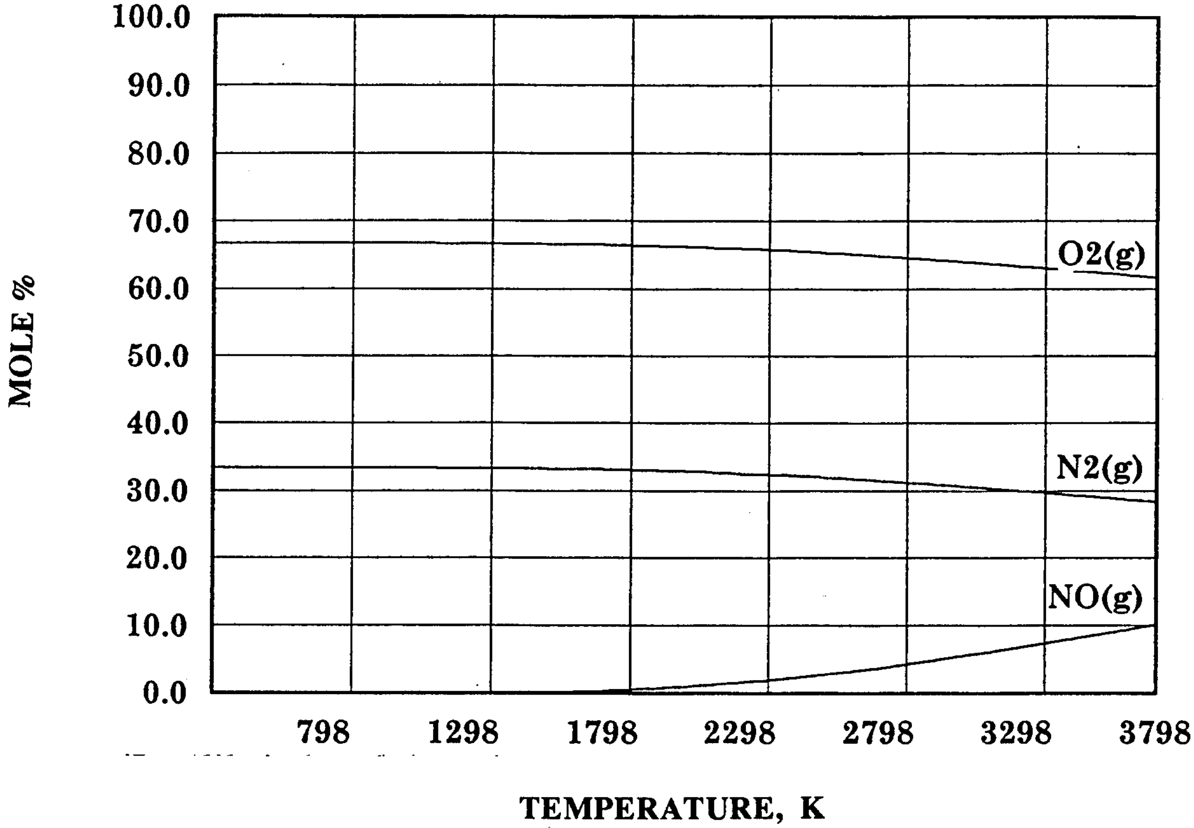

Figure 4. Equilibria Involving Nitric Oxide, Oxygen, And Nitrogen.

$$NO(g) \rightleftarrows \frac{1}{2}N_2\,(g) + \frac{1}{2}O_2(g)$$

B. RP-1/LIQUID OXYGEN

1. Rocket Propellant 1 (RP-1)

RP-1 is a kerosene fraction obtained in crude oil refining and hydrocarbon cracking and tailored by distillation to have a greater concentration of cyclic napthenic hydrocarbons and a lower concentration of paraffin hydrocarbons (Reference 13). The composition typically consists of 41 percent paraffins (n- and iso-), 56 percent napthenes, and three percent aromatics. No olefinic compounds are reported. The empirical formula used for rocket performance calculations is from $CH_{1.95}$ to $CH_{2.00}$. This fuel, as well as other petroleum based fuels, forms yellow-white brilliantly radiating flames and gives good engine performance. This formulation lends high temperature thermal stability, and has fewer engine deposits upon engine cooling. In addition, the melting point of naphthenic hydrocarbons with long side chains is lower than the melting point of normal paraffin hydrocarbons, and thus the napthenic hydrocarbons are more desirable as components of jet propellants and rocket propellants. The heat value of RP-1 is approximately 10,300 calories per gram. Two designations of this value are reported: a maximum heat value, determined using a calorimetric bomb by burning the substance in oxygen at one atmosphere pressure and allowing the combustion products to cool to 25°C, and a minimum heat value which is determined in the identical manner, but neglecting the heat evolved by the condensation of water vapor. The minimum heat value has been adopted as the standard value for hydrocarbon propellants.

Properties of a liquid propellant depend to a significant extent on volatility, i.e., the vapor pressure. Whereas aviation grade gasoline has a sufficient vapor pressure and can start an engine even as low as -60°C, the vapor pressure of RP-1 at 25°C is extremely low ($\approx$13 mm Hg). Volatility, and consequently, the ease of engine starting can be characterized by the temperature at which ten percent of the propellant vaporizes. For most kerosene-type propellants used in air breathing jet engines, this temperature is 175°C to 210°C. The temperature range for ten percent evaporation of RP-1 is 185°C to 210°C. Thus the combination of RP-1 with its oxidant source (liquid oxygen) requires an external ignition source, such as a hypergolic cartridge, to initiate combustion in the liquid rocket motor (Reference 14).

Engine starting depends mainly on physicomechanical factors, namely the volatility of the propellant and the degree of atomization. The latter property depends on the propellant's viscosity and surface tension, as well as the atomization system and the injection pressure. Heavy propellants with low vapor pressures typically require a greater degree of atomization than do light hydrocarbon propellants for ignition to occur. At a viscosity greater than 15 to 25 centistokes (25 cS = 20 cP for RP-1), good atomization of the propellant in the engine cannot be assured. A viscosity down to 25 cS at low temperatures is permitted in the specification of jet propellants. RP-1 has a viscosity of 1.5 cP at 25°C and 0.6 cP at 100°C, and should be well atomized under these conditions. Trimethyl aluminum, $Al(CH_3)_3$ and triethylaluminum, $Al(C_2H_5)_3$, are often added to hydrocarbon based propellants to reduce ignition delays.

2. Liquid Oxygen.

Liquid oxygen boils at 90 K, has a specific gravity of 1.14, and a heat of vaporization of 50.9 calories per gram. The standard heat of formation of oxygen gas at 25°C and one atmosphere pressure is 0 calories per mole by definition, but 3124 calories per mole are required to vaporize the propellant at the normal boiling point and to heat the gas products to 298 K (sensible heat). This value is therefore used for the heat of formation in most thermochemical calculations involving liquid oxygen. It is used in combination with alcohols, jet and rocket fuels, gasoline, and hydrogen. Although it does not spontaneously burn with organic materials at ambient pressures, liquid oxygen is considered incompatible with most carbon containing materials, and explosions have occurred when a confined mixture of oxygen and organic matter is suddenly

pressurized. Impact tests show that mixtures of liquid oxygen and hydrocarbon oils and other organic materials detonate violently. Liquid oxygen is a noncorrosive and nontoxic liquid and does not deteriorate materials of construction, if they are relatively clean. When in contact with human skin, the cryogenic propellant causes severe burns. Because liquid oxygen has a very high vapor pressure, it cannot be stored for extended periods of time without excessive losses due to evaporation, and all service systems using liquid oxygen (including propulsion systems) must be well insulated to preclude heat absorption which can accelerate vapor loss. Liquid oxygen is typically prepared by the rarefaction of air.

3. Bipropellant Reaction

The simple stoichiometric combustion reaction between RP-1 and liquid oxygen is shown below:

$$CH_2 + O_2\,(l) \rightarrow \frac{1}{3}\,CO_2 + \frac{1}{3}\,H_2 + \frac{2}{3}\,CO + \frac{2}{3}\,H_2O \qquad (19)$$

The amounts of carbon dioxide, carbon monoxide, hydrogen, and water vapor are those expected for burning the propellant under adiabatic conditions, neglecting the formation of high energy species (Reference 15). The heat of reaction for the simple reaction is $-7.81\text{x}10^4$ calories per mole. The reaction determined by rocket exhaust equilibrium programs[1] is shown in Equation (20)

$$1.046\ CH_{1.95} + 1.1877\ O_2(l) \rightarrow 0.7460\ CO + 0.3000\ CO_2 + 0.1469\ H + 0.2171\ H_2 + 0.6491\ H_2O + 0.0650\ O + 0.1604\ OH + 0.0775\ O_2 \qquad (20)$$

The heat of reaction from Equation (20) is $-6.215\ \text{x}10^4$ calories, and the adiabatic flame temperature is 3064 K. As discussed previously, several high energy chemicals are expected to recombine and form more thermodynamically stable products as the fireball is cooled, and the selection of the combustion reaction for atmospheric dispersion modeling is discussed in more detail in Section V. Thermal and physical properties for the RP-1/Liquid Oxygen System are presented in Table 3.

4. RP-1 Thermal Decomposition

Thermal decomposition of RP-1 occurs between 400°C and 600°C and is synonymous with petroleum cracking. In this event, higher alkane hydrocarbons are converted to lower alkanes, alkenes, and some hydrogen upon the application of thermal energy. The process yields predominantly ethylene (C_2H_4) together with other small molecules. The primary decomposition pathway for RP-1 is presented in Equation (21).

$$2\ CH_2 \rightarrow C_2H_4 \qquad \Delta H = +2.50\text{x}10^4 \text{ calories} \qquad (21)$$

This decomposition mechanism is endothermic, unlike decompositions of hydrazine and UDMH which are exothermic. Excess RP-1 in a fireball cloud would therefore result in cloud cooling as energy is absorbed during decomposition of the hydrocarbon propellant.

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[1]Beckhan, J.M. "Delta II Launch Vehicle Exhaust Data". Goddard Space Flight Center Memorandum. August 21, 1992.

5. RP-1 Oxidation

Residual RP-1 present in the fireball cloud reacts with oxygen from entrained air according to the following:

$$CH_2 + \frac{3}{2} O_2 (g) \rightarrow CO_2 + H_2O \quad \Delta H = -1.46x10^5 \text{ calories} \tag{22}$$

The heat release approximates the empirical heat content of 10,300 calories/gram. This reaction was used instead of the propellant combustion reaction presented in Equation (19) because it represents combustion with entrained air after cooling to ambient temperature. This process would be expected in a fireball as air is entrained and the cloud cools.

6. RP-1 Vaporization

Because RP-1 is a complex mixture of hydrocarbon fractions, some of which vaporize more readily than others, no single equation can properly describe the vaporization of this mixture. RP-1 has an initial boiling point of 180°C and boiling is complete at 263°C (Reference 16). The average vapor pressure at room temperature is very low (≈0.25 psia at 24°C). The heat of vaporization ranges from 40 - 95 calories per gram, with an average value of 58.6 calories per gram measured at the normal boiling point. Equation (23) represents the vaporization of RP-1 and provides an approximation of the true mass and thermal properties of the propellant. To properly model chemicals and not empirical formulas, the chemical selected for vaporized RP-1 was normal dodecane (n-$C_{12}H_{26}$), with a molecular weight of 170 grams per mole and a published heat of formation of the vapor of - 69526 calories per mole (Reference 17). Vaporized RP-1 is actually a mixture of normal and cyclical saturated alkane hydrocarbons.

$$CH_2 (l) \rightarrow \frac{1}{12} C_{12}H_{26} (g) \quad \Delta H_{vap,298} = +4.26x10^2 \text{ calories} \tag{23}$$

The calculated heat of vaporization is 30.6 calories per gram, somewhat lower than the values specified above, nevertheless the selection of n-dodecane provides a good match with the mass properties of RP-1. The molecular weight and density of n-dodecane (170 grams per mole and 0.749 grams per cubic centimeter, respectively) are similar to the average molecular weight and density of RP-1 (173 grams per mole and 0. 800 grams per cubic centimeter, respectively). The difference in the heat of vaporization can be attributed to two factors: the heat of formation of CH_2 liquid is lower per carbon atom than that predicted using straight chain aliphatic hydrocarbons[2], and the cycloparrafins (naphenes) have a higher net heat of vaporization per unit weight than the straight chain hydrocarbons. This difference is attributed to the packing geometry of the cycloparrafins in the liquid, which result in increased molecular attractive forces in the bulk liquid. The selection of n-dodecane was made to simplify the source model for the Delta II vehicle, and the difference in the thermal properties arising from this selection have minimal effects on the final thermal properties of the resultant fireball. Vaporized RP-1 in the final fireball cloud is expected to be less than one percent of the total amount of combustion gases and vaporized propellants in the cloud.

[2] $\Delta H_f \, CH_{1.95}$=-6220 calories per mole. Knear, C. (Lt. USAF Los Angeles Air Force Base), "Heat of Formation of RP-1". Private Communication. September 7, 1993.

TABLE 3. LIQUID PROPELLANT SOURCE DATA, RP-1/LIQUID OXYGEN BIPROPELLANT SYSTEM.

Propellant Type:	FUEL: RP-1	OXIDIZER: LOX	
Usage:	Booster Delta II		

PHYSICAL PROPERTIES

	Fuel	Oxidizer
Density:	0.800 g/cm^3 @ 298 K	1.149 g/cm^3 @ 90 K
Chemical Formula:	$CH_{1.95}$	O_2
Molecular Weight:	13.976 g/mole	31.999 g/mole
Vapor Pressure (Liquid)	≈0.25 psia (13 mmHg) @ 297 K	100 mmHg @ 74K

THERMAL PROPERTIES

	Fuel	Oxidizer
Heat of Formation, 298 K:	-6.220 kcal/mole	-3.124 kcal/mole*
Heat of Vaporization at T:	+58.6 cal/g @ NBP = 269°C	1.629 kcal/mole
Heat of Combustion:	-10380 cal/g	
Heat Capacity, Liquid:	0.429 cal/g-K @ -17.8°C	0.405 cal/g-K @ NBP 0.220 cal/g-K@293K 101.3 KPa

*Effective Heat of Formation

THERMODYNAMIC PROPERTIES OF COMBUSTION PRODUCTS

Component	Chamber	Exit Equil	Component	Chamber	Exit Equil
CO	31.58%		OH	6.79%	
CO_2	12.70%		O_2	3.28%	
H	6.22%				
H_2	9.19%				
H_2O	27.48%				
O	2.75%				

Adiabatic Flame Temperature 3064 K

C. SOLID PROPELLANTS

1. Generalized Combustion Scheme

Solid rocket propellants have been developed to be significantly heterogeneous in structure. Inorganic oxidizers such as ammonium perchlorate are dispersed throughout the binder which is a fuel source for the propellant. The binder typically consists of a natural rubber and plasticizer. Powdered aluminum metal is added to increase the heat transfer of the propellant mix and to serve as an additional fuel source. Other additives such as surfactants and catalysts are added to improve the casting properties and combustion stability of the propellant. The composition allows the propellants to be cast in a variety of sizes and shapes, which are tailored to meet thrust and mission profile requirements. A simple combustion reaction represented by solid propellants is depicted in Equation (24).

$$\frac{8}{5}NH4ClO4+\frac{6}{5}Al+3CH2 \rightarrow \frac{6}{5}CO2+\frac{9}{5}CO+\frac{2}{5}H2O+5H2+\frac{4}{5}N2+\frac{8}{5}HCl+\frac{3}{5}Al2O3(l) \qquad (24)$$

In Equation (24), CH_2 is intended to represent the reduced empirical formula for the main binder component of the solid rocket propellant. The heat of formation of CH_2 is +984 calories/mole, corresponding to the heat of formation of the binder used in the Titan IV solid rocket motors. The main combustion products are carbon dioxide, carbon monoxide, water vapor, hydrogen, nitrogen, hydrogen chloride and aluminum oxide. The heat of reaction of Equation (24) is -3.37×10^5 calories. Different formulations for solid propellants are made by varying the ratio of the three main ingredients, and by employing slightly different binder formulations. Titan IV Solid Rocket Motors (SRM) uses a United Technologies Chemical Systems Division formulation that employs polybutadiene acrylonitrile (PBAN) as the binder. Delta II Graphite Epoxy Motors (GEM) uses a formulation manufactured by Hercules which employs hydroxyterminated polybutadiene (HTPB) as the binder material. The Titan formulation additionally has iron oxide (Fe_2O_3), which serves as a catalyst for solid propellant combustion. The following sections describes these specific propellants in more detail.

2. Titan IV Solid Propellant

The solid propellant for the Titan IV Solid Rocket Motors (SRM) consists of the PBAN organic binder, metallized aluminum fuel and ammonium perchlorate oxidizer. The chemical structure for PBAN consists of a butadiene linkage with carboxyl (COOH) groups located at the end of each chain. A cyano group (CN) is included in the representation of the PBAN structure.

PBAN (approximate structure)

$$H-(CH_2-CH=CH-CH_2)_n-\left(\begin{array}{c}H\\|\\C\\|\\C\equiv N\end{array}-CH_2\right)_m-\left(\begin{array}{c}H\\|\\C\\|\\COOH\end{array}-CH_2\right)_p-H$$

$$m\approx 8;\quad n\approx 2;\quad p=1 \qquad (25)$$

A crosslinking agent consisting of the epoxy resin and anhydrides is used during the polymerization phase of PBAN processing at United Technologies Corporation. Cyanide ($C \equiv N$) is formed during this polymerization phase. Cyanide remains covalently bound to the solid propellant and may release hydrogen cyanide gas (HCN) in the event of an incomplete burn. For stoichiometric combustion, however, the cyanide breaks down into carbon monoxide (CO), carbon dioxide (CO_2) and oxides of nitrogen (NO_x). A representative combustion reaction for the Titan IV solid propellant formulation UTP-3001B[3] is presented in Equation (26).

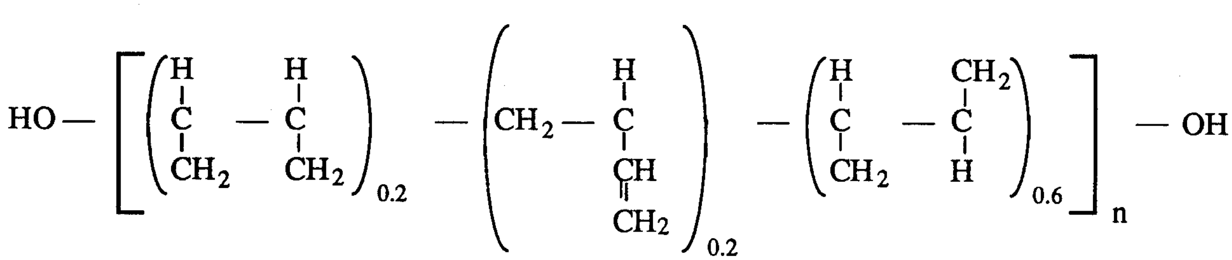
$$\begin{aligned} &NH_4ClO_4(s) + 1.0397\ Al(s) + 1.8407\ CH_{1.427}O_{.095}N_{.021}(s) + 0.0027\ Fe_2O_3(s) \rightarrow \\ &0.0401\ AlCl + 0.0114\ AlOCl + 1.7511\ CO + 0.0875\ CO_2 + 0.1416\ Cl + 0.5032\ H + \\ &0.8005\ HCl + 1.9318\ H_2 + 0.6955\ H_2O + 0.5178\ N_2 + 0.0600\ OH + 0.4874\ Al_2O_3(l) \\ &+0.0027\ Fe_2O_3(s) \end{aligned} \tag{26}$$

The heat of reaction for Equation (26) is -1.92×10^5 calories, and the adiabatic flame temperature is 3003 K, using a microcomputer-based chemical equilibrium program (Reference 18). In the above equation, the empirical formula representing the binder consists of the PBAN polymer, methyl nadic anhydride polymer, dioctyl adipate, and epoxy resin. The heat of formation of this empirical formula is -3434 calories/mole. As discussed in the previous liquid propellant section, the high energy chemicals (AlCl, AlOCl, Cl, H, OH) are expected to recombine after fireball cooling, and a more simple combustion reaction described in Section V will be used for modeling purposes. Table 4 presents the solid propellant source data for the Titan IV formulation. The heat of explosion listed in Table 4 was calculated assuming carbon reacts to form carbon monoxide, metals are oxidized to their highest normal oxidation state, chlorine reacts to hydrogen chloride gas, excess oxygen forms liquid water, excess hydrogen remains as elemental gas, and all nitrogen is present as diatomic nitrogen gas.

3. Delta II Solid Propellant

The solid propellant used in the graphite epoxy motor (GEM) for the Delta II launch vehicle consists of a hydroxyterminated polybutadiene (HTPB) binder, aluminized metal fuel, and an ammonium perchlorate solid oxidizer. HTPB consists of a butadiene carbon chain with a hydroxyl group at the end of the chain. The approximate chemical structure for the carbonaceous binder is shown below:

HTPB (approximate structure)



$n \approx 50$

(27)

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[3]Trowbridge, J.C. "Thermodynamic Information for UTP-3001B". United Technologies Chemical Systems. Internal Correspondence. Febuary 3, 1993.

TABLE 4. SOLID PROPELLANT SOURCE DATA, AP-PBAN-AL, TITAN IV FORMULATION.

Propellant Type: AP-PBAN-AL CPIA Unit No.: UTP-3001B

Manufacturer: United Technologies CSD Usage: Titan IV SRM

Loaded Weight: 591,000 lb/motor x2 motor = 1.182×10^6 lbs

PROPELLANT COMPOSITION

Constituent	Trade Name	Molecular or Empirical Formula	Formula Weight	Nominal WT%	$\Delta H°_f$ (cal/mole)
Ammonium Perchlorate	AP	NH_4ClO_4	117.49	67.51	-70690
Aluminum	Al	Al	26.984	16.12	0
Ferric Oxide		Fe_2O_3	159.69	0.25	-197000
Polybutadiene Acrylonitrile	PBAN	$CH_{1.4300}O_{0.0360}N_{0.0320}$	14.476	10.08	984
Methyl Nadic Anhydride	MNA	$C_{10}H_{10}O_3$	178.26	1.23	-106500
Dioctyladipate	DOA	$C_{22}H_{42}O_4$	370	2.42	-296000
Epoxy Resin	DER-332	$CH_{1.144}O_{0.1900}$	16.203	2.39	-11200

PHYSICAL PROPERTIES

Density (25°C): 1.760 g/cm^3 Flame Temperature at P=1atm: 3003 K

THERMODYNAMIC PROPERTIES:

Heat of Explosion (ΔH_{ex} cal/g): -1.46361×10^5 cal/100 g (calculated)

Heat Capacity C_p (cal/g-°C): Not Available

Heat of Formation ΔHf (cal/g) at 298K: -44568 cal/100 g

Empirical Formula (gm-atoms/100 g): $Al_{0.5974}C_{1.0565}Cl_{0.5746}Fe_{0.0031}H_{3.8062}N_{0.5969}O_{2.4030}$

THERMODYNAMIC PROPELLANT OF COMBUSTION PRODUCTS

(P_c = 1 atm)

Component	Chamber	Exit Equil	Component	Chamber	Exit Equil
AlCl	0.02306	moles/100 g	HCl	0.45998	
AlClO	0.00658		H_2	1.11002	
CO	1.00620		H_2O	0.39962	
CO_2	0.05028		N_2	0.29754	
Cl	0.08138		OH	0.03446	
H	0.28912		Al_2O_3 (l)	0.28008	

The products of the combustion of the HTPB propellant also include carbon dioxide, carbon monoxide, water vapor, hydrogen, nitrogen, hydrogen chloride, and aluminum oxide, although in different proportions. The combustion reaction for this solid propellant as determined by rocket exhaust equilibrium programs[4] is presented in Equation 28.

$$NH_4ClO_4(s) + 1.1987\ Al(s) + 1.3904\ CH_{1.622}(s) \rightarrow 1.2974\ CO + 0.0808\ CO_2 + 0.1958\ Cl + 0.0493\ AlCl + 0.7228\ HCl + 1.6113\ H_2 + 0.7451\ H_2O + 0.6469\ H + 0.4978\ N_2 + 0.1092\ OH + 0.5493\ Al_2O_3(l) \quad (28)$$

The heat of reaction for Equation 24 is -1.94×10^5 calories, and the adiabatic flame temperature is 3152 K, again calculated using the microcomputer equilibrium program. The binder represented in Equation (28) is a composite empirical formula having an effective heat of formation of -4241 calories/mole. This composition includes contributions from the HTPB, liquid aromatic aziridine bonding agent (HX-752), di(2-ethylhexyl) sebacate (DOS), triphenylbismuth (TPB), dimethyldiisocyanate (DDI), maleic anhydride (MA), 2,2' methylene bis (4 methyl - 6 tert-butyl phenol), and tri (mixed mono- and di-nonyl) phenyl phosphite. Table 5 presents the solid propellant source data for the Delta II formulation.

D. PROPELLANT INTERACTIONS

In addition to the propellant combustion reactions discussed above, during the evolution of a fireball cloud combustion products resulting from the various types of liquid and solid rocket propellants may mix and produce unique chemicals. Identification of possible chemicals resulting from the mixing of combustion gases from the Aerozine-50/nitrogen tetroxide liquid propellant system and the PBAN solids are documented in Reference 19. Other possible propellant interactions are discussed below.

1. RP-1 and Nitrogen Tetroxide

Reactions between vaporized RP-1 and N_2O_4 can have three distinct reactive pathways: complete oxidation, partial oxidation, and nitration.

a. Complete Oxidation

Nitrogen tetroxide is a chemical oxidizer and is likely to react or even explode upon contacting organic materials. Tests conducted at the Martin Marietta Chemical Technology Laboratory[5] demonstrated that the mixing of a small amount of nitrogen tetroxide liquid with a paraffinic oil containing a carbon length of ≈ 20 (Shell Oil Company Turbo-T-220) resulted in a rapid pressure and temperature rise indicative of an exothermic reaction. A postulated reaction between excess RP-1 fuel, expressed as n-dodecane, and nitrogen tetroxide oxidizer is presented in Equation 29.

$$C_{12}H_{26}(g) + \frac{37}{4} N_2O_4(g) \rightarrow 12\ CO_2 + \frac{37}{4} N_2 + 13\ H_2O \quad (29)$$

[4]Bodrero, T.A. "Thermochemical Calculations for QDL Propellant". Hercules Aerospace Company Memorandum. January 18, 1993.

[5]Simon, E. "Effect of Hot Autogeneous Gases on Fuel/Oil and Oxidizer/Oil Mixtures". Martin Marietta Space Systems Interoffice Memorandum. August 4, 1991.

TABLE 5. SOLID PROPELLANT SOURCE DATA, AP-HTPB-AL, DELTA II FORMULATION.

Propellant Type: AP-HTPB-AL CPIA Unit No.: QDL

Manufacturer: Hercules Usage: Delta II GEM

Loaded Weight: 25,800 lb/motor x 9 motor = 2.322×10^5 lbs

PROPELLANT COMPOSITION

Constituent	Trade Name	Molecular or Empirical Formula	Formula Weight	Nominal WT%	ΔH°_f (cal/mole)
Ammonium Perchlorate	AP	NH_4ClO_4	117.49	69.60	-70690
Hydroxyterminated Polybutadiene	HTPB	$CH_{1.622}$	13.646	11.24	-4241
Aluminum	Al	Al	26.982	19.16	0

PHYSICAL PROPERTIES

Density (25°C): 1.8019 g/cm^3 Flame Temperature at P=1atm:3152K

THERMODYNAMIC PROPERTIES:

Heat of Explosion (ΔH_{ex} cal/g): -1.64353×10^5 cal/100 g (calculated)

Heat Capacity C_p (cal/g-°C): 178.817 cal/100 g

Heat of Formation ΔHf (cal/g) at 298K: -45368 cal/100 g

Empirical Formula (gm-atoms/100 g): $Al_{0.7042}C_{0.8164}Cl_{0.5873}H_{3.6738}N_{0.5939}O_{2.3960}$

THERMODYNAMIC PROPELLANT OF COMBUSTION PRODUCTS

(P_c = 1 atm)

Component	Chamber	Exit Equil	Component	Chamber	Exit Equil
AlCl	0.02921	moles/100 g	HCl	0.4282	
CO	0.7686		H_2	0.9545	
CO_2	0.04784		H_2O	0.4414	
Cl	0.1160		N_2	0.2949	
H	0.3832		OH	0.06467	
			Al_2O_3 (l)	0.3254	

The calculated heat of reaction for Equation (29) is -1.83×10^6 calories. The prevalence of this reaction in an accident involving the Delta II vehicle is unknown, and would depend on the degree of mixing between the two types of liquid rocket propellants. Because the mass loading of the RP-1/LOX bipropellant system (212,900 total pounds) is quite large as compared to the Aerozine-50/nitrogen tetroxide bipropellant system (13,399 total pounds), this interaction is expected to have a negligible effect on the final chemical composition of the fireball cloud.

b. Partial Oxidation

An incomplete oxidation of paraffinic and branched hydrocarbons may also occur, and various carbonyl compounds (aldehydes, ketones, and carboxylic acids) may form. For example, the reaction of methane with N_2O_4 at 440°C-680°C in the presence of various catalysts yields formaldehyde in somewhat low (under 25 percent) yields. Undecane yielded a mixture of fatty acids, from which pelargonic acid can be isolated.

c. Nitration

In addition to the above two mechanisms, direct nitration of paraffins may occur with nitrogen tetroxide. In the nitration of propane with nitrogen tetroxide at 790°C, approximately equal quantities of nitromethane, nitroethane, 1-nitropropane, and 2-nitropropane forms (Reference 20). In addition to the nitroparaffins mentioned, miscellaneous oxidation products include acids and aldehydes. A large percentage of starting materials does not react. Hydrocarbons from n-pentane through n-nonane are effectively nitrated with nitrogen tetroxide at 200°C. This results in mixtures of mononitroderivatives, $CH_3(CH_2)_nNO_2$, and dinitroderivatives $O_2NCH_2(CH_2)_nNO_2$, with conversions of 30 - 80 percent depending on the conditions. When cyclohexane reacts with nitrogen tetroxide diluted with carbon dioxide (one hour at 10 - 80°C), a 15 percent yield of mononitrocyclohexane forms.

Nitrate and carbonyl groups initially form from Exxon Primol 355 oil , a mixture of paraffins and cyclic napthalenes[6]. Nitro compounds which also form are insensitive to decomposition at elevated temperatures.

A postulated mechanism for the nitration of RP-1 (expressed as n-dodecane) is presented in Equation (30). As previously discussed, the extent of nitration in an actively growing fireball is dependent on mixing conditions, and is therefore difficult to predict.

$$2\,C_{12}H_{26}(g) + \frac{3}{2}N_2O_4(g) \rightarrow 2\,C_{12}H_{25}NO_2 + NO + H_2O \tag{30}$$

2. RP-1 and Hydrogen Chloride

Because of growing environmental and health concerns with chlorinated hydrocarbons, possible chlorination of RP-1 from hydrogen chloride launch gases was investigated.

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[6]Damschen, P.E. "Nitration of Primol by N_2O_4". Interoffice Memorandum. Space Division, Air Force Systems Command.

The accepted mechanism for the preparation of alkyl halides occurs by exposing the hydrocarbon to halogen gas at elevated temperatures in the presence of ultraviolet light. Under the influence of ultraviolet light at 250°C - 400°C, methane and chlorine react vigorously to produce hydrogen chloride (HCl) and chloromethane (CH_3Cl) (Reference 21). The reaction also produces in a series of chlorinated analogues of methane in accordance with Equation (31).

$$CH4 \xrightarrow{X2} CH3X \xrightarrow[+HX]{X2} CH2X2 \xrightarrow[+HX]{X2} CHX3 \xrightarrow[+HX]{X2} CX4 \quad (31)$$

X = Br, Cl, I
light or heat required

Chlorination of aliphatic hydrocarbons in the absence of ultraviolet irradiation has not been reported in the literature, and a proposed mechanism represented in Equation (32) is very endothermic.

$$CH_4(g) + HCl(g) \rightarrow CH_3Cl(g) + H_2(g) \quad (32)$$

The calculated heat of reaction is +1.99x10^4 calories. When the Gibbs free energy for this reaction is calculated, values of 2.05 x 10^4 calories and 1.93 x 10^4 calories are obtained at 298 K and 2900 K, respectively. 2900 K is a reasonable fireball temperature. At these temperatures, the calculated equilibrium constant is low (9.09x10^{-16} at 298 K and 3.53 x 10^{-2} at 2900 K), and therefore this reaction is not thermodynamically favored at the temperatures expected for a launch vehicle explosion.

Chlorinated hydrocarbons, may however form from the addition of chlorine free radicals. These radicals form in the high temperature combustion of solid rocket propellants specified in Equations (26) and (28). The stepwise mechanism for the formation of chlorinated hydrocarbons from free radical addition is shown below

$$\begin{aligned} &HCl \xrightarrow{heat,UV} Cl\cdot + H\cdot \\ &2Cl\cdot \rightarrow Cl2 \\ &Cl\cdot + CH4 \rightarrow HCl + CH3\cdot \\ &CH3\cdot + Cl2 \rightarrow CH3Cl + Cl\cdot \end{aligned} \quad (33)$$

The chlorination of residual RP-1 is possible via this mechanism. Chlorination is expected to be regulated by kinetic factors and the shifting chemical equilibrium of the combustion gases as the fireball cloud cools. Chlorinated hydrocarbons were observed from propellant interaction tests (Reference 22), but these were attributed to the incomplete combustion of the PBAN solid propellant.

The addition of hydrogen halides to alkenes to form alkyl halides is also a viable reaction mechanism.

$$C_2H_4 + 2HCl \rightarrow 2CH_3Cl \quad (34)$$

Chlorination of RP-1 is also possible via this mechanism, because the primary thermal decomposition product of RP-1 is ethylene (C_2H_4). Because chlorinated hydrocarbons were absent on completion of the propellant combustion tests between RP-1 and the GEM solid rocket propellant, the formation of chlorinated hydrocarbons will not be used in source modeling. The reactions are, however, technically feasible via free radical addition and by addition to ethylene.

3. Nitrogen Tetroxide and Hydrogen Chloride.

Nitrogen tetroxide and hydrogen chloride react to form nitric acid and nitrosyl chloride in accordance with Equation (35).

$$N_2O_4(g) + HCl(g) \rightarrow HNO_3(g) + NOCl(g) \quad (35)$$

This reaction is thermodynamically favored at all temperatures between ambient (298 K) and expected fireball temperatures (2900 K). The Gibbs free energy for this reaction at 2900 K is -20315 calories/mole (-85 kJ/mole) (References 23,24). Mixing of solid propellant combustion products with liquid propellant combustion products is expected to occur during a launch vehicle accident. The formation of nitrosyl chloride is therefore expected from a launch vehicle accident employing nitrogen tetroxide and solid rocket propellants. The incorporation of this chemical reaction into the chemical source model is discussed further in Section V.

4. Other Pertinent Reactions

Other propellant reactions, such as the reaction between hydrazine and ammonium perchlorate to form hydrazinium perchlorate ($N_2H_5ClO_4$), the reaction between hydrazine and hydrogen chloride to form hydrazinium chloride (N_2H_5Cl), and the reaction between nitrogen dioxide and ammonia to form ammonium nitrate (NH_4NO_3), are examples of several other chemical reactions which may occur during fireball growth. These particular chemicals are, however, thermally unstable and are expected to decompose to their precursers or elemental constituents at the high temperatures within the fireball cloud. Liquid nitrogen tetroxide and liquid oxygen may also react with the solid propellant fuel sources available (aluminum, PBAN, HTPB) to initiate combustion. Although the combustion products predicted from the mixing of solid and liquid rocket propellants are not significantly different than the products expected from the propellants acting alone (Reference 23), any reaction between the solid and liquid rocket propellants should provide sufficient heat to ignite the solid propellants and sustain the burning. This indicates that a significant failure mechanism for a fully loaded launch vehicle would be a liquid spill or leak which contacts the solid propellant.

E. INTERACTIONS WITH AIR

In addition to the myriad of reactions discussed above, reactions between the chemicals released from a launch vehicle accident and the atmospheric components of air are possible, after the fireball cools and is dispersed by prevailing winds. Although a complete analysis of these interactions are outside the scope of this effort (this contract is limited to the description of fireball properties up to the point of fireball burnout), a brief discussion is warranted. As discussed previously, the exact chemical composition resulting from an accident is temperature-, and thus time-dependent. Several chemicals react with oxygen, atmospheric water vapor, and carbon dioxide at ambient temperature. Many of the reactions discussed below have been verified in laboratory tests performed as part of this contract, and these data provide a more complete representation of the fate of combustion products and unreacted rocket propellants in the atmosphere. Research continues in the atmospheric chemistry of vaporized propellants[7], and results from these studies should provide a more complete understanding of these unique processes.

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[7]Lundblad, Bart. The Aerospace Corporation. Private Communication. January 28, 1994.

1. Combustion Reactions

After mixing with air and upon cooling, fireball components may react with entrained oxygen as shown in Table 6.

TABLE 6. AFTERBURNING REACTIONS EXPECTED DURING FIREBALL DISPERSION AND COOLING.

Fireball Component	Reactive Path		Notes
CO	$CO + \frac{1}{2}O_2 \rightarrow CO_2$	(36)	favored below 3300 K
H_2	$2H_2 + O_2 \rightarrow 2H_2O(g)$	(37)	favored at all temperatures*
NO	$NO + \frac{1}{2}O_2 \rightarrow NO_2$	(38)	favored below 765 K
NH_3	$2NH_3 + \frac{3}{2}O_2 \rightarrow N_2 + 3\,H_2O(g)$	(39)	favored at all temperatures*
CH_4	$CH_4 + 2O_2 \rightarrow CO_2 + 2\,H_2O(g)$	(40)	favored at all temperatures*
C_2H_4	$C_2H_4 + 3\,O_2 \rightarrow 2\,CO_2 + 2\,H_2O(g)$	(41)	favored at all temperatures*
$C_{12}H_{26}$	$C_{12}H_{26}(g) + \frac{37}{2}\,O_2 \rightarrow 12\,CO_2 + 13\,H_2O(g)$	(42)	favored at all temperatures*

* Evaluated between 298 K and 4000 K

Although the reactions in Table 6 are all thermodynamically favored (negative Gibbs free energy) as the fireball cloud cools to ambient temperature, kinetic factors must also be considered. Methane concentrations in air, for example, form explosive mixtures in concentrations between 5 to 15 percent by volume and an ignition source is required to initiate combustion. The equilibrium between carbon monoxide and carbon dioxide (Equation 36) indicates that reversion to the relatively nontoxic dioxide is expected at ambient temperature. Carbon monoxide is however kinetically stable at room temperature. Thermodynamic equilibria compositions for this reaction are shown in Figure 5. Water vapor formed in the above reactions will condense until the vapor-phase composition is at its equilibrium value (3.1 volume percent at 298 K).

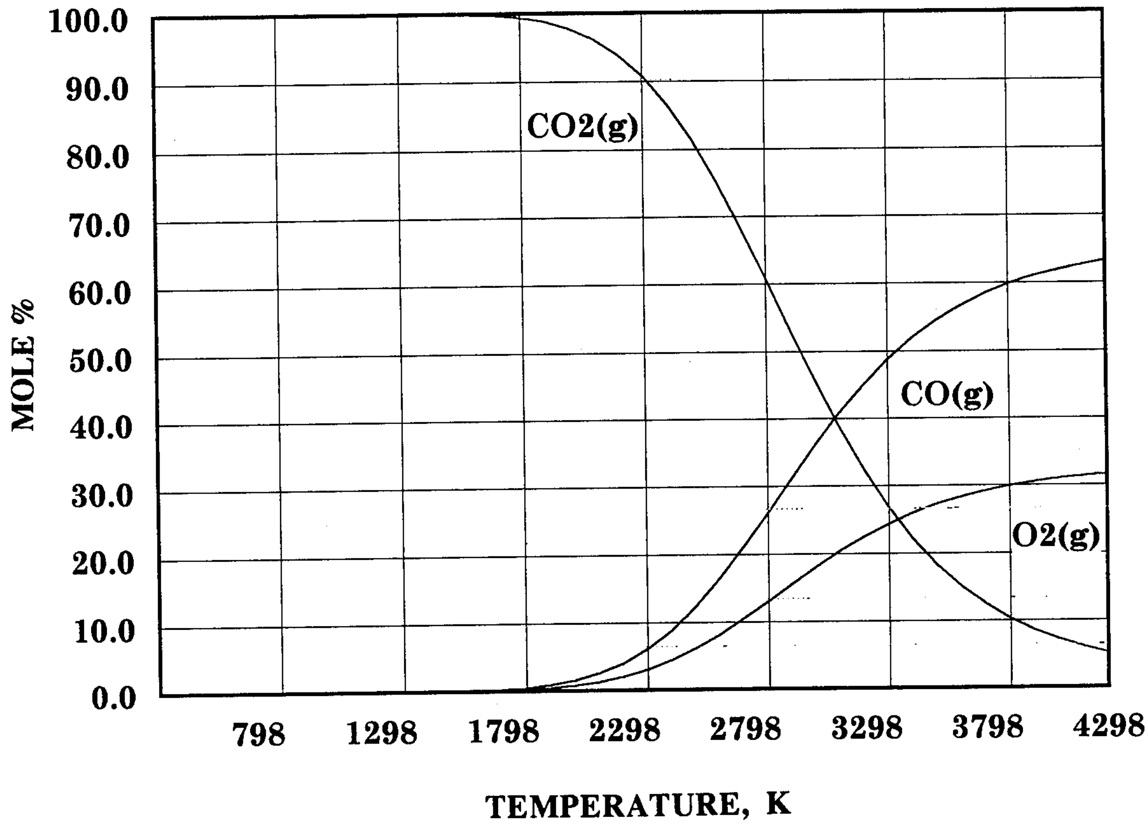

Figure 5. Equilibria Involving Carbon Monoxide, Carbon Dioxide, And Oxygen

$CO + \frac{1}{2}O_2 \rightleftarrows CO_2$

2. Aerozine-50 Reactions

Ambient temperature reactions between Aerozine-50 and air are complicated and are being studied by a number of investigators. A previous study by this author (Reference 25) recommended the use of the following reactions with corresponding half-lives for atmospheric decay processes. These reactions were evaluated in Pyrex® gas sampling bulbs, and the heterogeneous reacton rates determined under these conditions were significantly higher than expected homogeneous gas-phase reactions.

$$N_2H_4(g) + O_2 \rightarrow N_2 + 2\ H_2O(g) \qquad t_{\frac{1}{2}} = 5 \text{ hours} \tag{43}$$

$$3\ C_2H_8N_2(g) + 2O_2 \rightarrow 2\ C_3H_8N_2 + 4\ H_2O + N_2 \qquad t_{\frac{1}{2}} = 46 \text{ hours} \tag{44}$$

$$C_2H_8N_2(g) + O_2 \rightarrow C_2H_6N_2O + H_2O \qquad t_{\frac{1}{2}} = 0.2 \text{ hours} \tag{45}$$

The atmospheric reaction of hydrazine with oxygen (Equation 43) produces water vapor and molecular nitrogen. Equation (44) is the predominant heterogeneous atmospheric decay reaction with molecular oxygen for unsymmetrical dimethylhydrazine ($C_2H_8N_2$). Two moles of formaldehyde dimethylhydrazone ($C_3H_8N_2$) as well as water vapor and nitrogen form from this reaction. Approximately 99.8 percent of the UDMH is removed in accordance with this reactive path. The remaining amount of UDMH (0.2 percent) forms N-nitrosodimethylamine ($C_2H_6N_2O$) and water vapor in accordance with Equation (45). Although produced in minor amounts, NDMA is cancer producing, and is a concern for launch vehicle abort modeling. These reactive half-lives were measured in humid air, and considerably longer times were recorded for conditions in which dry air was used.

Many past efforts (References 26,27,28) in which decay mechanisms for hydrazine and UDMH with dry and humid air have been reported originated from heterogeneous wall-catalyzed reactions. To minimize the influence of wall effects, small surface-to-volume ratio reaction chambers were constructed using chemically inert Teflon® film. These chambers produced hydrazine decay results which were characterized by adsorption onto and permeation through the fluorocarbon wall rather than by chemical oxidation. A study in a 5615 liter fluorocarbon chamber with a surface-to-volume ratio of 3.39 m^{-1} demonstrated that the half life of a 100 ppm hydrazine sample in dry air was identical to that in dry nitrogen (Reference 29). The same author reported that metallic wall materials, such as aluminum, galvanized steel, stainless steel, titanium, or corroded aluminum dramatically increased the rate of disappearance of the hydrazines. This finding may explain the inability to recover excess unreacted propellants in a 150 liter stainless steel chamber thirty minutes after propellant combustion tests have been completed (Reference 30). The ultimate environmental fate of the hydrazines was dictated by reaction with atmospheric ozone, catalyzed reactions with oxygen on the surfaces of particulate matter, and reactions with other minor atmospheric constituents. Reactions of hydrazine with moderately polluted atmospheres containing ozone, hydrocarbons, and nitrogen oxides occurred in less than two hours, due to reactions with ozone and hydroxyl radicals.

The homogeneous reaction between hydrazine and molecular oxygen was presumed by other researchers (Reference 31) to be very slow, if it occurred at all. Stone (Reference 32) reinforced the concept that the major reaction pathways for hydrazine fuels was via atmospheric pollutants, including ozone and nitrogen dioxide. Decay rates were rapid under these conditions and noxious compounds including diazine, ammonia, nitrosodimethylamine, tetramethyltetrazine, formic acid, and ammonia were formed.

In addition to the decay mechanisms with molecular oxygen, hydrazine and UDMH may also react with carbon dioxide to form hydrazine carboxylic acid and dimethylcarbozate, respectively (Reference 33). These reactions probably do not occur at high temperatures:

$$N_2H_4 + CO_2 \rightarrow NH_2NHCOOH \quad (46)$$

$$C_2H_8N_2 + CO_2 \rightarrow (CH_3)_2NNHCOOH \quad (47)$$

3. Reactions with Atmospheric Water Vapor.

The kinetics of the gas-phase reaction between nitrogen dioxide and water vapor was studied by England and Corcoran (Reference 34). In this study, nucleation and condensation of nitric acid into liquid phase mists occurred above 50 ppm HNO_3 at one atmosphere pressure and 25°C. The reaction produced both nitric and nitrous acids, and nitrous acid reacted with additional oxygen to reform nitrogen dioxide. The overall reaction in the presence of oxygen is represented in Equation (48). The gas-phase reaction of NO_2 with water vapor is a fast, homogeneous reaction that initally follows third order kinetics. The initial rate of reaction increases as the square of the nitrogen dioxide concentration, and increases linearly with the water vapor concentration. The reaction is therefore slow at low NO_2 concentrations and very fast at high NO_2 concentrations. The half life for this reaction at an NO_2 concentration of 50 ppm and a one percent water vapor concentration is less than 0.2 hours (12 minutes). For an initial concentration of 10 ppm of nitrogen dioxide, the half-life for reaction is about 5 hours.

$$4\,NO_2 + 2\,H_2O + O_2 \rightarrow 4\,HNO_3 \qquad R^0_{NO_2} = -k(NO_2)^2(H_2O) \quad (48)$$

Other researchers have investigated the heterogenous reaction between nitrogen dioxide and water vapor. A half life for the reaction of nitrogen dioxide with water vapor in a stainless steel chamber was reported to be 2.5 hours[8]. The test conditions were T = 70°F, $[H_2O] = 5000$ ppm (19 percent relative humidity at 72°F), $[NO_2]_{initial} = 250$ ppm. When the same reaction mixture was performed in a Teflon chamber, the half-life varied from 19.2 hours to 28.2 hours depending on the surface-to-volume ratio.

Theoretical studies performed by the Lawrence Livermore National Laboratory (Reference 35) suggest that the reaction between nitrogen dioxide and water vapor in the proper proportions forms an azeotropic mixture:

$$4\,NO_2 + 8.432\,H_2O + O_2 \rightarrow 4\,(HNO_3 + 1.608\,H_2O) \quad (49)$$

These results indicate that when nitrogen dioxide vapors are released into the atmosphere, misting and condensation of liquid-phase nitric acid occurs if the concentration is elevated above 50 ppm NO_2.

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[8]Giordano, T. "Evaluation of Kinetics of Reaction of Nitrogen Tetroxide with Water Vapor". Martin Marietta Memorandum. August 25, 1992.

SECTION IV

FAILURE MODES, MIXING CHARACTERISTICS, AND CONTINUED REACTIONS

Properly defining the failure modes, mixing, and reaction characteristics of a launch vehicle explosion is essential to the characterization of the resulting chemical and thermal environments. The failure mode is the sequence of events that describes a particular catastrophic launch vehicle accident. The mixing and reaction characteristics are a function of vehicle type, propellant loading, and failure mode. These characterists are used to define the thermochemical environment of the ensuing fireball. The methods used to determine mixing and reaction characteristics, as well as the analytical results, are discussed in this section.

A. FAILURE MODES

As used in this study, vehicle failure mode is the general type of failure which results in the complete destruction of the vehicle. Vehicle configuration, altitude, and velocity are considered components of the vehicle failure mode. The root or component level cause of the failure is not important to this study because it does not alter the predictions made using the general type of vehicle failure.

The process of identifying failure modes for the launch vehicles of interest (Titan II, Delta II, and Titan IV) follows these guidelines:

An identified failure mode must be generalized. Only major system level failures are considered.

An identified failure mode must be supported by existing data. Most of the failure modes identified in this report are based on the Project Pyro investigation (Reference 4).

An identified failure mode must be considered credible by the range safety community.

High-velocity impacts are not considered credible failures for these launch vehicles. These vehicles would be destroyed by actuation of a range safety destruct command before a high velocity impact with the ground surface could be attained.

1. Titan II Failure Modes

The following credible failure modes have been identified for the Titan II launch vehicle.

a. Command Destruct

This failure mode results when the range safety officer sends a command destruct signal to the vehicle as a result of an aberrant trajectory or upon the indication of immediate vehicle failure or danger. This signal initiates the destruct package on the vehicle and ensures complete destruction.

b. Confined by Ground Surface (CBGS)

This failure mode represents those failures of a fully fueled vehicle which occur prior to or at launch ignition. In this scenario, liquid rocket propellants are released onto the ground surface and react there. This type of failure includes, but is not limited to, mechanical failure of one or more of the propellant tanks due to over-pressurization, failure due to structural weak spots, or failure by mechanical intrusion or flaws. This type of failure could also be initiated by a fire on the pad or by other environmental causes (extremely high winds, lightning strikes, earthquake, etc.)

c. Low Velocity Impact (LVI)/ Fallback onto the Pad

This failure mode represents those failures that lead to the loss or significant reduction of thrust or guidance within the first several seconds of flight. As a result of this type of failure, the launch vehicle would contact the ground surface near the launch pad at a relatively low velocity. Failures of this type include, but are not limited to, turbopump failure, nozzle failure, propellant supply system failure, nozzle actuator failure, and guidance control failure.

2. Titan IV Failure Modes

The following credible failure modes have been identified for the Titan IV launch vehicle.

a. Command Destruct/ Inadvertent Separation Destruct System (ISDS)

This failure mode results when the range safety officer sends a command destruct signal to the vehicle as a result of an aberrant trajectory, the indication of immediate vehicle failure or danger, or evidence of early separation as monitored by the onboard ISDS. Any of these events initiates the in-flight destruct package on the vehicle, which ensures the complete destruction of the vehicle. The ISDS continuously monitors several critical vehicle interfaces, such as the Solid Rocket Motor (SRM) to core vehicle interface and the stage one to stage two interface. If an early separation in any of the interfaces is detected, the ISDS initiates a vehicle destruct action. The Titan 34D-9 accident in 1986 resulted from the ISDS actuation of the destruct package.

b. Confined by Ground Surface (CBGS)

This failure mode represents those failures of a fully fueled vehicle which occur prior to or at launch ignition. Liquid propellants are released onto the ground and react there, and the solid propellants fracture and burn on the ground. Failures of this type include, but are not limited to, mechanical failure of one or more propellant tanks due to over-pressurization, weak spots, other mechanical intrusions, or the inadvertent ignition of one of the SRMs. This type of failure could also be initiated by a fire on the pad or by other environmental causes (extremely high winds, lightning strikes, earthquake, etc.)

c. Low Velocity Impact (LVI)/ Fallback onto the Pad

This failure mode represents those failures that lead to the loss or significant reduction of thrust or guidance within the first several seconds of flight. As a result of this type of failure, the launch vehicle would contact the ground surface near the launch pad at a relatively low velocity. Failures of this type include, but are not limited to, failure of one SRM to ignite, early SRM burst or burn-through, nozzle failure, Thrust Vector Control (TVC) system failure, and guidance control failure.

d. SRM Failure

This failure mode represents catastrophic failures of one or both of the solid rocket motors. This type of failure can thrust the vehicle off-course, cause very hot gases to impinge upon the core vehicle, or cause the structural failure of the SRM. All of these scenarios may result in a launch vehicle explosion. Possible causes of this type of failure include, but are not limited to, premature burn-through of the solid rocket motor due to a crack, debond, or void in the solid grain, segment interface failure, or loss of all or part of the nozzle. This type of failure generally leads to the initiation of the in-flight destruct system by the ISDS or the Range Safety Officer. Both the Titan 34D-9 and Titan IV K-11 accidents were attributed to failures of the solid rocket motors.

3. Delta II Failure Modes

The following credible failure modes have been identified for the Delta II launch vehicle.

a. Command Destruct

This failure mode results when the range safety officer sends a command destruct signal to the vehicle as a result of an aberrant trajectory or upon the indication of immediate vehicle failure or danger. This signal initiates the in-flight destruct package on the vehicle and ensures the complete destruction of the vehicle.

b. Confined by Ground Surface (CBGS)

This failure mode represents those failures of a fully fueled vehicle which occur prior to or at launch ignition. Liquid propellants are released onto the ground and react there, and the solid propellants fracture and burn on the ground. This type of failure includes, but is not limited to, mechanical failure of one or more propellant tanks due to over-pressurization, weak spots, structural failure, other mechanical intrusion, and the inadvertent ignition of one or more of the Solid Motors. This type of failure could also be initiated by a fire on the launch pad or by other environmental causes (extremely high winds, lightning strikes, earthquake, etc.)

c. Low Velocity Impact (LVI)/ Fallback onto the Pad

This failure mode represents those failures that lead to the loss or significant reduction of thrust or guidance within the first several seconds of flight. As a result of this type of failure, the launch vehicle would contact the ground surface near the launch pad at a relatively low velocity. Failures of this type include, but are not limited to, ignition failure of one or more of the six ground ignited solid motors, turbopump failure, liquid motor nozzle failure, propellant supply system failure, nozzle actuator failure, guidance control failure, early solid motor burst or burn-through, solid motor nozzle failure, and guidance control failure.

d. Graphite Epoxy Motor (GEM) Failure

This failure mode represents a catastrophic failure of one or more of the nine solid rocket motors on the Delta II vehicle. This type of failure can thrust the vehicle off course, cause very hot gases to impinge upon the core vehicle, or cause the structural failure of the solid motor. All of these scenarios could lead to a launch vehicle explosion. Possible causes of this type of failure include, but are not limited to, premature burn-through of the GEM due to a crack, debond, or void in the solid grain, or loss of all or part of the nozzle. This type of failure generally results in the initiation of the Range Safety Destruct System.

e. Confined by Missile

This failure mode represents flight failures resulting in the catastrophic breakup of the core (liquid propellant portion) vehicle. This type of failure results in inadvertent mixing of the liquid fuels and oxidizers and the complete destruction of the vehicle. Possible causes of this type of failure include, but are not limited to, propellant tank dome failure, intertank failure, or failures of other structural elements.

B. INITIAL MIXING

The first step in determining the propellant participation during a launch vehicle accident is to define the quantity of propellants involved in the initial explosive event. This event occurs during the first 3 - 20 milliseconds after ignition of the command destruct pyrotechnic charges. To define the propellant participation, overpressure results of the Project Pyro investigation (Reference 4) were taken, propellant quantities were related to these overpressures, and results were adapted to the physical configurations of the launch vehicles of interest.

During the early 1960's, a large-scale test program (Project Pyro) was undertaken to define the overpressure and thermal environments resulting from the unintentional mixing of liquid rocket propellants. Some of the limitations of the Project Pyro test program data were:

All testing was conducted on single pairs of propellant tanks, rather than on multiple sets of tanks now found on the majority of launch vehicles.

Very few large-scale tests were performed, especially with hypergolic liquid rocket propellants.

Limited thermal data were obtained.

The data were highly variable and introduced a significant statistical uncertainty its use.

In spite of these limitations, Project Pyro supplied the best and only significant data derived from the large-scale testing of propellants and configurations of interest to this study.

Most of the data reported by Project Pyro are in the form of trinitrotoluene (TNT) equivalents for each type of propellant and failure mode investigated. TNT equivalency is defined as the quantity in pounds of TNT required to produce the same overpressure as the liquid propellants, at a given distance from the explosion. The TNT equivalency of liquid propellants varies with the distance from the center of explosion. The overpressure-distance curves for TNT and liquid propellants have different shapes close to the explosion, but converge at greater distances. The standard method used to determine TNT equivalencies for propellants is to measure the far-field overpressures where the pressure-distance curves converge. The TNT equivalency determined from far-field overpressure is called the Terminal Yield. Table 7 presents Terminal Yield data for the propellants and failure modes investigated in this study.

TABLE 7. PROJECT PYRO OVERPRESSURE DATA SUMMARY.

HYPERGOLIC PROPELLANTS:		
Failure Mode	**Terminal Yield**	**Upper Limit**
CBGS	0.02% - 0.3%	0.5%
Command Destruct	0.3% - 0.35%	0.5%
Low Velocity Impact/ Fallback	1.5%	5.0%
Small Explosive Donor	0.8% - 1.2%	2.0%
LOX/RP-1		
CBM & Command Destruct	10% for L/D > 5 *	N/A
CBGS & Low Velocity Impact	4.0% - 12.0% **	N/A

*L/D= Length to diameter ratio of the propellant tanks
**A function of impact velocity. As impact velocity increases, Terminal Yield increases
N/A = Not Applicable

Equating overpressure/terminal yield data to the quantity of propellants reacted is a simple matter of comparing the theoretical thermochemical energy released per pound of TNT to the theoretical thermochemical energy released per pound of propellants. This method assumes that the propellants involved react stoichiometrically, which is probably not the case. For nitrogen tetroxide/Aerozine-50, the ratio of propellant energy to TNT energy is 2.4 (Reference 36). For the propellant combination of LOX/RP-1, the ratio of propellant energy to TNT energy is 1.23.

1. Titan IV Initial Mixing Model

The initial mixing model developed for a command destruct failure of a Titan IV launch vehicle was based upon the following scenario and assumptions. Figure 6 includes a graphical description of the scenario.

When the destruct package is initiated, the quantity of propellants reacted during the first 3 - 5 milliseconds corresponds to the Project Pyro command destruct data. These reactions occur at the interface between the Stage 1 intertank and the Stage 2 intertank.

After the initial event, additional reactions occur at the interface between the Stage 1 oxidizer tank and the Stage 2 fuel tank. These reactions result from the force of the initial explosions which drive the propellant masses together, are treated as small explosive donors, and occur between 5 and 20 milliseconds after initiation of the command destruct signal.

The entire mass of oxidizer contained in the 13-inch internal feed lines reacts with the surrounding fuel due to the degree of confinement of the oxidizer.

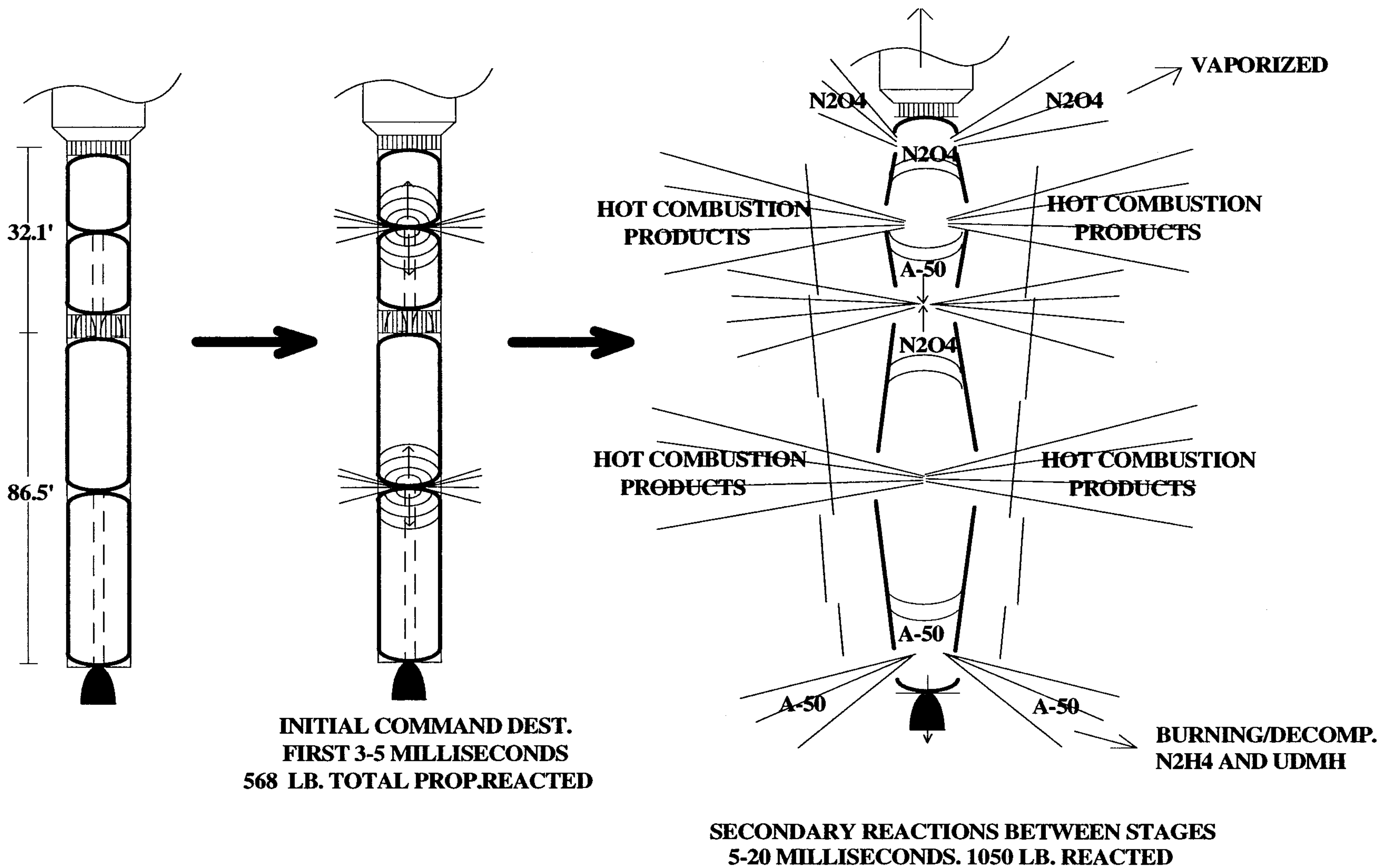

Figure 6. Titan IV Core Vehicle Command Destruct.

For flight altitudes of interest to this program (0-10,000 feet) the Titan IV vehicle does not consume any of its core vehicle propellants. Only the two, Stage 0 solid rocket motors burn during the first phase of a Titan IV launch. The following propellant weights are expected to react during the initial 20 milliseconds after initiation of the command destruct pyrotechnic charges.

First 3 to 5 ms.: (341,000 pounds Stage 1 propellants + 77,000 pounds Stage 2 propellants) * 0.00325/2.40=568 total pounds liquid propellants reacted (50)

Where: 0.00325 is the average Terminal Yield for a command destruct accident employing hypergolic rocket propellants and 2.40 is the ratio of propellant energy to TNT energy.

From 5 to 20 ms: (224,000 pounds Stage 1 oxidizer + 27,900 pounds Stage 2 fuel) * 0.01/2.40 = 1050 total pounds liquid propellants reacted (51)

Where: 0.01 is the average Terminal Yield for small explosive donors and employing hypergolic liquid rocket propellants

From the oxidizer feed lines, 3.14159 * (0.5417 feet)^2 *59 feet * 89.47 pounds/feet^3= 4866 pounds N_2O_4 react stoichiometrically with 2550 pounds of Aerozine-50, to provide a total mass of reacted propellants equivalent to 7416 pounds.

The mass of propellants which react during the first 20 milliseconds of a Titan IV command destruct abort is 9034 pounds, or 2.16 percent of the initial liquid propellant mass.

Identical analyses were performed for the remaining abort and vehicle configurations. Results of these analyses are presented in Table 8.

TABLE 8. INITIAL PROPELLANT REACTION RATIOS BY VEHICLE TYPE AND FAILURE MODE.

VEHICLE	FAILURE MODE	PROPELLANTS REACTED
TITAN IV	Command Destruct	2.16% or 9034 lb.
TITAN IV	SRM Failure	2.19% or 9173 lb.
TITAN IV	CBGS/Spill	1.93% or 8086 lb.
TITAN IV	Low Velocity Impact/Fallback	3.27% or 13,701 lb.
TITAN II	Command Destruct	2.16% of remaining A50/N_2O_4
TITAN II	CBGS/Spill	1.93% or 6086 lb.
TITAN II	Low Velocity Impact/Fallback	3.27% or ~10,313 lb.
DELTA II	Command Destruct	8.13 % of remaining LOX/RP-1 1.46% or 195 lb. A-50/N_2O_4
DELTA II	CBGS/Spill	9.75 % of remaining LOX/RP-1 0.125% or 17 lb. A-50/N_2O_4
DELTA II	SRM Failure	8.13 % of remaining LOX/RP-1 1.46% or 195 lb. A-50/N_2O_4
DELTA II	Low Velocity Impact/Fallback	9.75 % of remaining LOX/RP-1 0.625% or 85 lb. A-50/N_2O_4
DELTA II	Confined By Missile	8.13 % of remaining LOX/RP-1 1.4% or 187 lb. A-50/N_2O_4

C. CONTINUED BURNING REACTIONS

Reactions occurring after the first 20-120 milliseconds of an abort (duration of explosive event varies with propellant mass) and up to fireball burnout are attributed to the continued burning phase of an active fireball. The continued burning reactions have a greater effect on the resulting toxic cloud than reactions occurring during the initial explosive event. However, very little data have been reported for this portion of the fireball time history. Continued burning reactions are not supported by direct analytical treatment. The complexity of the phenomena and the large number of initial conditions and outside forces have a significant impact on the analysis. To perform a theoretical analysis, the number of assumptions and initial conditions makes the analysis invalid for most accidents. Lacking this information, a new method to describe this fireball regime was developed.

Once analytical modeling was eliminated, an analysis of existing empirical data was performed. Using these data in conjunction with propellant thermochemistry, models of continued burning reactions were developed. Development of the models assumed that the Project Pyro thermal data was reasonably accurate, and that there were no scaling factors in the application of this model to larger propellant quantities.

1. Continued Reaction in a LOX/RP-1 Fireball

The approach selected for modeling the continued burning reaction of a LOX/RP-1 fireball was based on the thermal data obtained during the large scale (25,000 pound) Project Pyro tests. The quantity of propellants which reacted to produce the thermal environment was determined by combining the LOX/RP-1 thermal data with a thermochemical model, and performing an overall energy balance on the fireball.

The first step of the analysis was to determine the heat flux per unit area for the LOX/RP-1 fireball. The Project Pyro large-scale LOX/RP-1 thermal test data from the 335 foot station were used for this purpose. The graphical data (Reference 4) were digitized, and a curve fit for the mean, maximum, and minimum heat flux were generated. The non-linear curve fit equations generated were:

a. Mean: $Q= 501.97*\tau^7-1964.35*\tau^6+3131.92*\tau^5-2160.56*\tau^4 +1211.1*\tau^3 -307.114*\tau^2+37.321*\tau+0.064$ (52)

b. Maximum: $Q= -5515.54*\tau^8+23973.5*\tau^7-43237.4*\tau^6+41733.5*\tau^5 -23173.1*\tau^4+7407.91*\tau^3-1296.64*\tau^2+108.613*\tau-0.04738$ (53)

c. Minimum: $Q= -263.899*\tau^8+917.388*\tau^7-1172*\tau^6+625.43*\tau^5 -71.59*\tau^4-48.8813*\tau^3+11.5462*\tau^2+2.00095*\tau-0.0016513$ (54)

Where:

Q= Heat flux per unit area, Watts/cm^2

τ= Dimensionless time, time from ignition (seconds) / fireball duration (seconds)

Figure 7 contains a graph of the mean data and the resulting curve fit. A correlation of 0.98 was obtained from this non-linear regression.

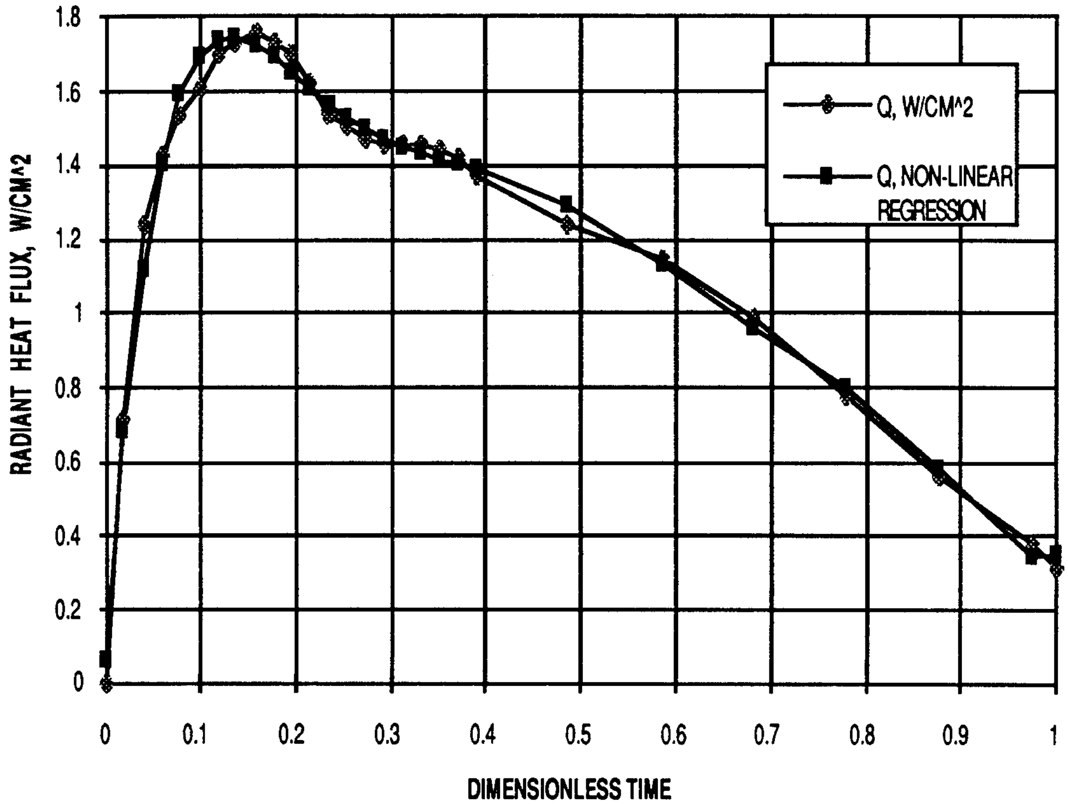

Figure 7. Data and Curve Fit for Heat Flux vs Dimensionless Time Measurements, LOX/RP-1, Pyro 25,000 Pound Tests, 335 Foot Station.

The second step of the analysis was to determine the effective emissivity of the fireball at the 335 foot station. It was assumed that the maximum recorded heat flux corresponded to the LOX/RP-1 adiabatic flame temperature, 2822 K. The maximum reported radiation was Q_{max}=3.34 W/cm^2 (33400 W/m^2) at a dimensionless time of 0.097. Using the equation for radiative heat transfer ($Q=\varepsilon\sigma AT^4$ where ε= emissivity (unknown), σ=5.67032 $*10^{-08}$ W/m^2*T(K)^4, and A= surface area, m^2), and using Qmax for Q/A , 2822 K for T, and solving for ε yields:

$$\varepsilon= Q/(\sigma AT^4)= 33400 \text{ W/m}^2/(5.67032*10^{-08}*2822^4) = 0.00929 \qquad (55)$$

0.00929 was the effective emissivity of the LOX/RP-1 fireball at the 335 foot monitoring station. Using the derived emissivity and the mean measured radiation at fireball burnout (0.32 W/cm^2), the fireball temperature at burnout was then determined.

$$T(\text{burnout})= (3200 \text{ W/m}^2 / (.00929*5.67032*10^{-08}))^{0.25} = 1570 \text{ K} \qquad (56)$$

Integrating the mean heat flux equation from t = 0 to burnout and multiplying by the effective surface of radiation at the 335 foot instrumentation stations, the total energy radiated from the fireball was calculated. The mean energy radiated from the 25,000 pound LOX/RP-1 test was $1.988 * 10^7$ BTU. These and other subsequent calculations are presented in Appendix A.

The fireball temperature, chemical composition, and heat capacity can be used to calculate the energy content of the fireball at burnout. The sum of the radiated energy, the energy content of the fireball at burnout, and the energy required to vaporize the liquid propellants is the total energy released by the reacted propellants. Using these values in the overall energy balance makes the analysis conservative. The energy expended in producing dynamic gas overpressures is not included in the analysis, and inclusion of this term is expected to yield a lower percentage of propellants reacted.

The next step of the analysis uses the expected stoichiometry for the LOX/RP-1 fireball to determine the percentage of propellants that reacted during the active burning phase to produce the reported energy. The stoichiometry assumed for this analysis is:

$$1.188\ O_2 + 1.046\ \text{RP-1 (as } CH_{1.95}) \Rightarrow 0.3\ CO_2 + 0.746\ CO + 0.614\ H_2O + 0.235\ H_2 + 0.195\ OH + 0.147\ H + 0.065\ O + 0.078\ O_2 \quad (57)$$

The reactant ratios used in this equation are based on a Delta II Stage 1 nominal loading. This stoichiometry yields a heat of reaction of -7870.6 BTU per pound of RP-1. The average heat capacity (C_p) of the fireball gases is 0.460 BTU/lb-R. This stoichiometry assumes no air entrainment into the fireball which is a conservative assumption.

Comparing the actual amount of energy released during the 25,000 pound tests ($4.358 * 10^7$ BTU), and the total energy content of the propellants if fully reacted ($9.838 * 10^7$ BTU), the percentage of propellants reacted to form the fireball is determined. This calculation accounts for the energy released during the initial mixing phase and continued burning phase of the fireball. Propellants reacted after fireball burnout are not considered in this analysis.

$$\text{Percent reacted} = (4.358 * 10^7 / 9.838 * 10^7) * 100 = 44.3\ \% \quad (58)$$

This analysis predicts that approximately 44 percent of the initial propellants in a LOX/RP-1 launch abort will react between t=0 and fireball burnout. This analysis, and its results, are only as accurate as the Project Pyro thermal data and the accompanying assumptions. Project Pyro data were obtained during tests that occurred during the late 1960's. These data did not have the accuracy or the documentation required of current test disciplines.

2. Continued Reactions in a Hypergolic Propellant Fireball

The approach used to model the continued burning phase of a hypergolic propellant fireball was similar to that used for the LOX/RP-1 fireball. The identical analysis could not be performed because of the lack of far-field thermal radiation data for large-scale Project Pyro tests. The only significant thermal data taken during the large scale hypergol tests was thermal heat flux measurements taken near the center of the fireball. These data were used in the continued burning analysis for hypergolic propellants.

Project PYRO tests 257 and 258 were both conducted with 1000 pounds of hypergolic propellants (A-50/N_2O_4) and were the largest scale hypergolic tests conducted during the Pyro program. Heat flux data from stations 257H, 257S, 258H, and 258S were used for this analysis. A plot of these data, including the mathematical mean, is presented in Figure 8.

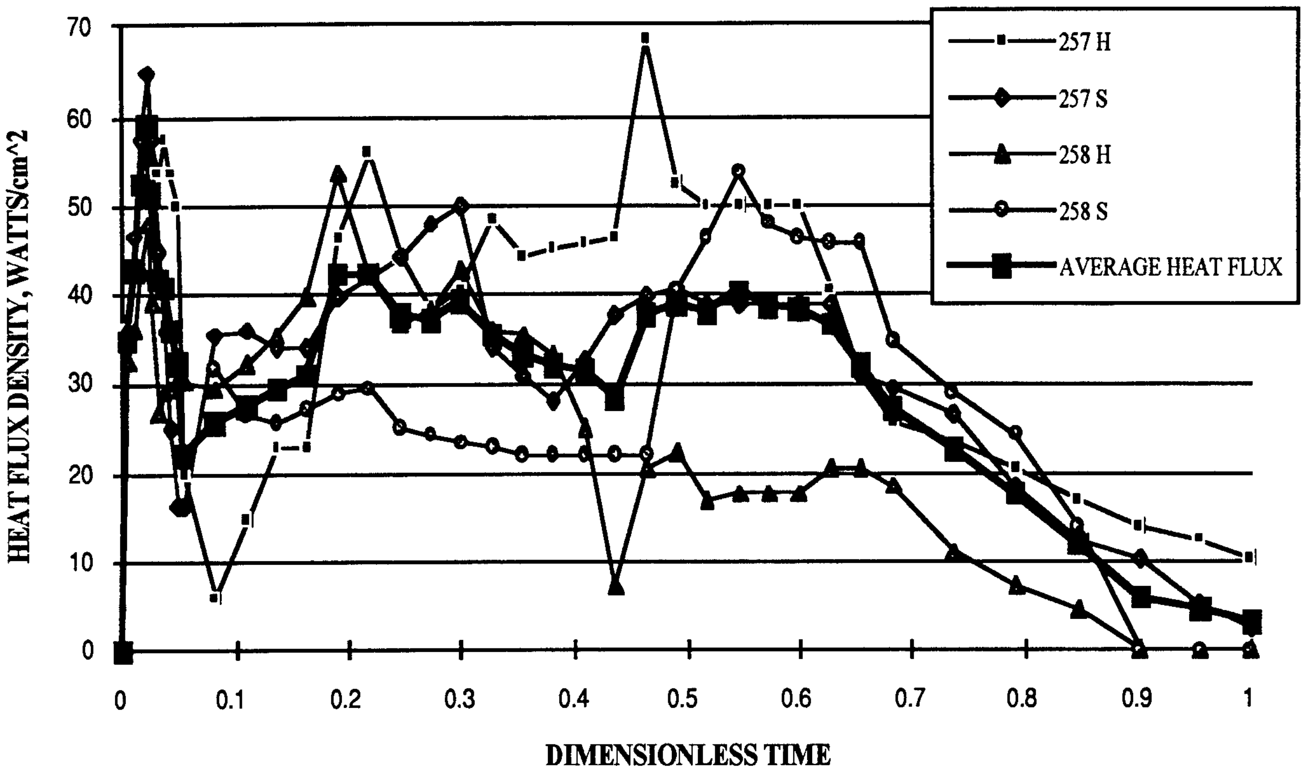

Figure 8. Heat Flux Data from Project Pyro 1000 Pound Hypergol Tests 257 and 258. (100 Foot Drop Tests).

Two distinct phases of heat flux are apparent within the fireball. All four data stations show a pronounced thermal pulse during the initial 120 milliseconds (dimensionless time = 0.055), and a decaying thermal environment of lower magnitude for the remaining 2.2 seconds (0.945 dimensionless time). The duration of the initial mixing/explosive event for a 1000 pound hypergolic accident coincides with the initial thermal pulse seen in this data (~120 ms), and the initial thermal spike likely results from the explosive mixing of the propellants. The initial thermal pulse recorded during the first 120 milliseconds of fireball growth is used in this analysis to describe the initial explosive mixing of the hypergolic propellants.

The quantity of propellants reacted during the initial mixing event is estimated using TNT equivalent overpressure data. For an 80 feet per second high velocity impact, project Pyro estimates that the TNT equivalence is five percent (Reference 37). Since the theoretical maximum TNT equivalence for A-50/N_2O_4 is 240 percent (Reference 36), the percentage of propellants reacted during the initial explosive event is (0.05/2.40)*100=2.1 percent, or 21 pounds. From this calculation, the initial heat flux pulse observed in the Pyro data results from 21 pounds of propellants reacting hypergolically.

By comparing the heat flux generated during the initial mixing phase of the fireball with the heat flux generated during the continued burning phase of the fireball, an approximation of the extent of continued burning is made. The first step of the analysis generates curve fit equations for the two phases of heat flux using the mean heat flux curve. Figures 9 and 10 present the mean heat flux data and the curve fit for the initial pulse and the continued burning pulse, respectively.

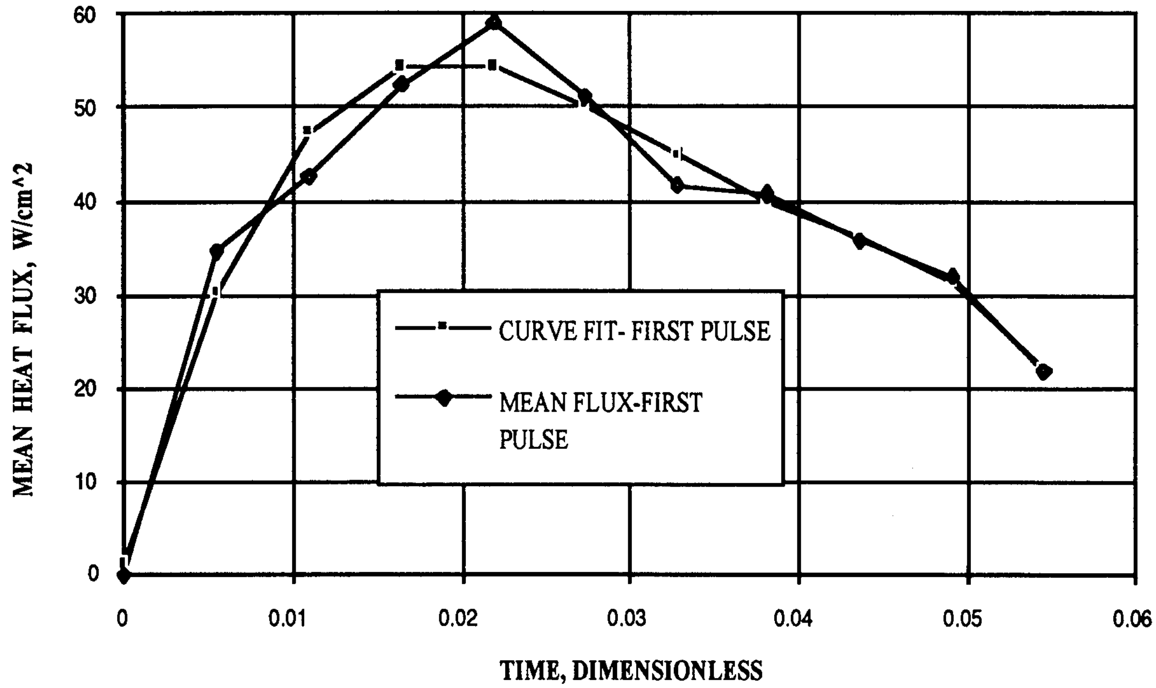

Figure 9. Mean Heat Flux Data and Curve Fit of the 1000 Pound Hyperglic Propellant 100 Foot Drop Tests - Initial Thermal Pulse.

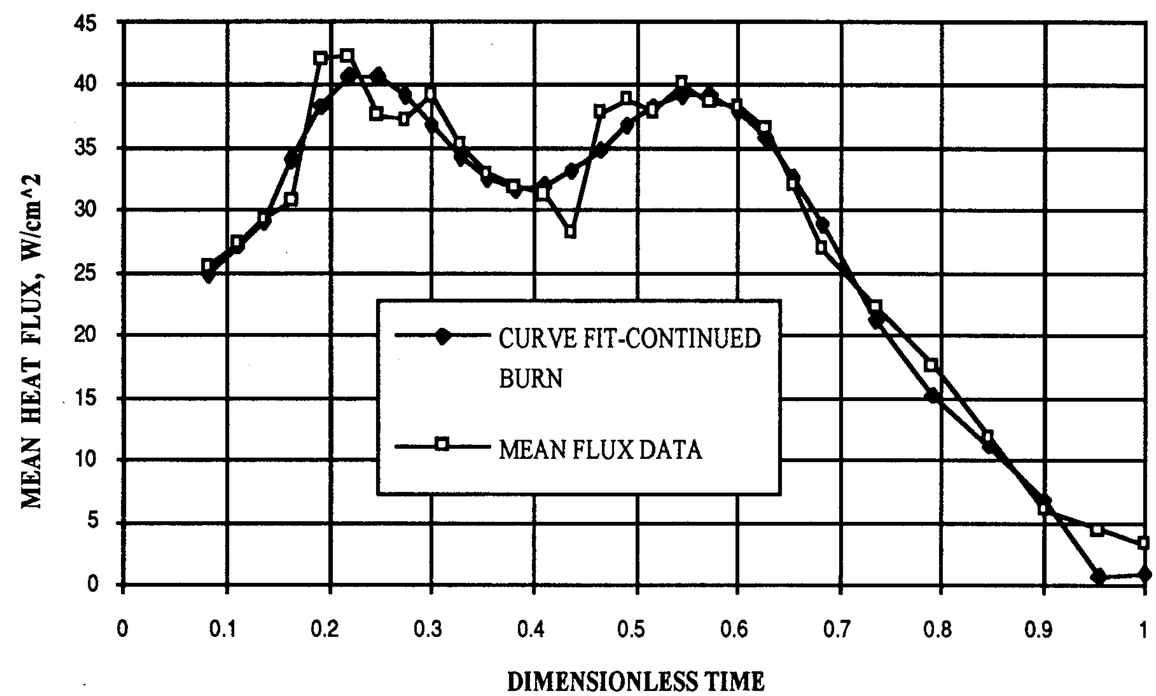

Figure 10. Mean Heat Flux Data And Curve Fit Of The 1000 Pound Hypergolic Propellant 100 Foot Drop Tests- Continued Burning Thermal Pulse.

The curve fit of the data is very good, with a correlation of better than 97 percent. The curve fit equation generated for the initial burning thermal pulse is:

$$Q(t) = -8.93413*10^8 (\tau)^5 + 8.06087*10^7 (\tau)^4 + 295856 (\tau)^3 -223999(\tau)^2 +6552.75(\tau) + 1.16313 \quad (59)$$

The curve fit equation generated for the continued burning thermal pulse is:

$$Q(t) = 1.97738 (\tau)^8 -895028 (\tau)^7 +1.68502 *10^6 (\tau)^6 - 1.70584 *10^6(\tau)^5 +.00264(\tau)^4 - 344804 (\tau)^3 + 66385 (\tau)^2 - 6371.67 (\tau) + 261.522 \quad (60)$$

Where:

$Q(t)$ = Heat Flux as a function of time, Watts/cm^2

$\tau = t/t_o$ = Dimensionless time, equals 1 at fireball burnout

t = time into event, seconds

t_o = fireball duration

Integrating Equation (59) from $\tau = 0$ to $\tau = .055$ yields a scaled heat release of 2.336. Integrating equation 60 from $\tau = 0.056$ to $\tau = 1$ yields a scaled heat release of 37.16. These calculations indicate that 15.9 times more energy was released during the continued burning phase of the fireball than was released during the initial explosive phase. Appendix A contains a MathCad® spreadsheet of these calculations. Since 21 pounds of propellants react to produce the initial thermal pulse, then the thermal equivalent of 333.9 pounds of propellant react during the continued burning phase of the fireball.

Although the calculations indicate that 333.9 pounds of propellant react during the continued burning phase of the fireball, not all of the energy results from reactions between A-50 and N_2O_4. In addition to hypergolic combustion, hydrazine monodecomposition and UDMH thermal decomposition may contribute to the observed thermal release. The amount of propellant reacted hypergolically is required to determine the extent of N_2O_4 reaction. To determine this parameter, the following assumptions are made about the fireball reactions:

No air is entrained into the fireball during active fireball growth.

All excess N_2H_4 undergoes monodecomposition.

95 percent of the excess UDMH undergoes thermal decomposition.

An iterative solution is performed to determine the extent of hypergolic reaction required for the thermal environments measured in the Project Pyro tests. The iterative solution consists of the following steps:

a. Determine the energy released by 333.9 pounds of hypergolic propellants reacting stoichiometrically. This is the quantity of total energy required during the continued burning phase of the reaction.

b. Provide an initial estimate of the percent of liquid propellants reacting hypergolically.

c. Calculate the total energy released by (1000-21 = 979) pounds of hypergolic propellants using the estimate provided in step (b), and using the prior assumptions.

d. Compare the total energy released in step (c) with the expected energy predicted in step (a). If the energy released is smaller than the expected energy, use a higher estimate for step (b) and repeat the calculations. If the energy released is larger than the expected energy, use a lower estimate for step (b) and repeat the calculations.

e. Continue the iterative calculations until the energy released is identical to the expected energy. This yields the percent of propellants reacted hypergolically. Using a fully loaded Titan IV launch vehicle as an example, the following values are generated using the iterative procedure outlined above.

f. If the entire mass of propellants reacts hypergolically, 2.08×10^{11} calories are released. Since only the thermal equivalent of 33.39 percent of the propellants react during the continued burning phase, the expected energy release is 6.95×10^{10} calories. Table 9 contains the reaction stoichiometry, mass balance, and heat release obtained from this calculation.

g. After several iterations, convergence of the expected energy with the released energy is attained. The amount of propellants reacted hypergolically corresponding to this final iteration is approximately 22 percent. A graph of these data is included in Figure 13.

TABLE 9. STOICHIOMETRY, HEAT AND MASS BALANCE FOR 100% REACTED HYPERGOLICALLY CASE.

CONSTITUENT	PROPELLANT QUANTITY, POUNDS	MASS PERCENTAGE OF TOTAL
Initial Loading		
N_2H_4	64,430	15.39
$C_2H_8N_2$	64,430	15.39
N_2O_4	289,340	69.22
Total	418,000	100.00
Reactants		
N_2H_4	64,430	15.39
$C_2H_8N_2$	64,430	15.39
N_2O_4	289,340	69.22
Total	418,000	100.00
Combustion Products		
CO_2	42,743	10.21
CO	32,949	7.87
H_2O	115,893	27.70
H_2	2,229	0.53
N_2	171,257	40.93
H	554	0.13
NO	7,045	1.68
O	5,011	1.20
O_2	23,738	5.67
OH	17,020	4.07
Total	418,439	99.99
Total Energy Released (calories)	2.08×10^{11}	

TABLE 10. % REACTED HYPERGOLICALLY Vs % OF EXPECTED ENERGY.

% REACTED HYPERGOLICALLY	% OF EXPECTED ENERGY PRODUCED
2.1	53.7
10	72.95
15	84.7
20	96
21	98.2
22	101.17

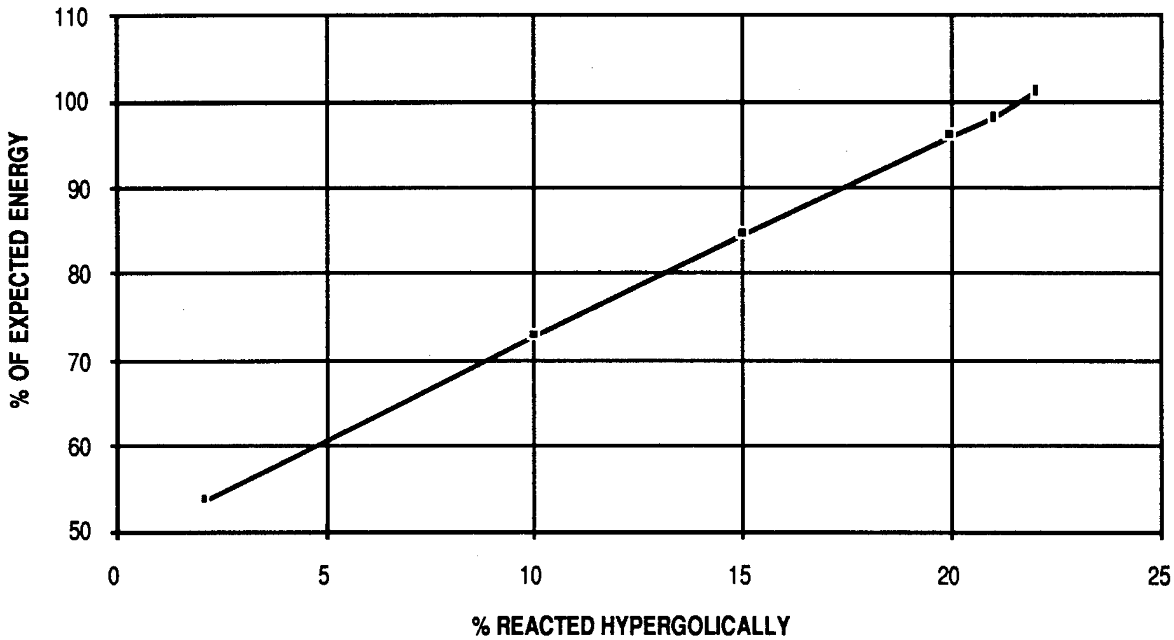

Figure 11. Graph of Table 10 Data.

The exact solution to the energy balance, in which all of the expected energy is attained, occurs between 21 percent and 22 percent of the propellants reacted hypergolically. The reaction stoichiometry, mass balance, and heat released for this situation is presented in Table 11.

TABLE 11. STOICHIOMETRY, MASS, AND THERMAL BALANCE OF THE 21% REACTED HYPERGOLICALLY CASE.

CONSTITUENT	PROPELLANT QUANTITY, POUNDS	MASS PERCENTAGE OF TOTAL
Initial Loading		
N_2H_4	64,430	15.39
$C_2H_8N_2$	64,430	15.39
N_2O_4	289,340	69.22
Total	418,000	100.00
Reactants		
N_2H_4	13,529	15.41
$C_2H_8N_2$	13,533	15.41
N_2O_4	60,733	69.17
Total	87,798	99.99
Combustion Products		
CO_2	8,976	2.14
CO	6,919	1.65
H_2O	24,338	5.82
H_2	468	0.11
N_2	35,964	8.60
H	116	0.03
NO	1,498	0.36
O	1,053	0.25
O_2	4,985	1.19
OH	3,574	0.85
Decomposition Products		
NH_3	27,047	6.47
H_2	1,601	0.38
N_2	45,973	10.99
CH_4	27,173	6.50
Vaporized Propellants		
N_2O_4	228,623	54.65
Total	418,308	99.99
Total Energy Released (calories)	7.22×10^{10}	

Twenty one percent of the initial hypergolic propellant mass reacts hypergolically during the continued burning phase of the fireball. Most of the excess hydrazine fuels also undergoes exothermic decomposition. These calculations are only as accurate as the empirical heat flux data taken during the Project Pyro test series and the assumptions made during the analysis. The database used for this analysis is limited, and may not be reliable or applicable to a wide range of failure modes and tank sizes. However, until further large-scale hypergol testing is completed, these data and the accompanying analyses serve the present study quite well. This analysis is conservative due to range safety requirements. Points of conservatism include:

a. Radiative heat losses from the fireball were not available or included in this analysis. Exclusion of these heat losses lowers the total energy predicted and the percent of propellants reacted.

b. Heat flux transducers were located near the fireball center. As a result, the measured heat flux was lower than the actual heat flux during the later stages of fireball growth. This was attributed to the buoyant rise of the fireball away from the transducers. Chemical reactions were also expected to occur away from the fireball center at the later stages of fireball growth.

SECTION V

THERMOCHEMICAL ANALYSIS

Accidental mixing of liquid rocket propellants (Aerozine-50, nitrogen tetroxide, RP-1, and liquid oxygen), or premature ignition and unstable combustion of the solid rocket propellants (Titan IV SRM or Delta II GEM) could result in destruction of the launch vehicle or solid motors, the release of considerable thermal energy, and the emission of combustion gases and vaporized propellants into the atmosphere. Accurate estimates of fireball thermal energies and chemical compositions are required to predict downwind concentrations of toxic chemicals to protect military and civilian populations in the accident vicinity. This section discusses the determination of chemical source emissions arising from an accident involving rocket propellants fueling the Titan II, Delta II, and Titan IV missile systems.

A. FLAME TEMPERATURE AND CHEMICAL COMPOSITION

Computer programs used to calculate complex chemical equilibrium compositions and rocket performance during steady-state flight do not allow for non-equilibrium ignition and combustion during a launch vehicle explosion. In the latter case, unreacted vaporized propellants and thermodynamically unstable reaction products may form due to kinetic barriers in the combustion reactions. During incomplete combustion, the product mixture retains its high chemical energy, and the average temperature of the resultant gases is lower. The decrease in temperature results in a lower cloud stabilization height, and a higher concentration of chemicals deposited at ground elevation. The combination of non-equilibrium combustion conditions (in which excess liquid propellants remain unreacted) and a lower cloud temperature (in which ground-level chemical deposition is greater) substantially increase the toxic hazards of a launch vehicle explosion over those predicted from a nominal launch.

Although vaporized liquid propellants (hydrazine, unsymmetrical dimethylhydrazine, nitrogen tetroxide, and RP-1) have a higher Gibbs free energy than their decomposition products (nitrogen, elemental carbon, hydrogen, and oxygen), the inefficient mixing and unconfined expansion of the propellant mixture result in discontinuities in the thermal equilibrium equations used to describe the system. Photographic evidence taken from the 1986 Titan III accident, as well as results from chamber propellant combustion tests performed under this contract, indicate that a substantial quantity of unreacted nitrogen tetroxide is released during an abort. The case for stoichiometric propellant mixing resulting in the attainment of thermodynamic equilibria may indeed be the exception rather than the rule. This is borne out by the difficulty and precise machining necessary to atomize and impinge propellants in modern liquid rocket engines (Reference 38). The identification and quantification of unreacted propellants and other chemicals not predicted by equilibrium computer programs is important because many of these chemicals are highly toxic. The relationships describing the contribution of these chemicals to the fireball are developed in the following sections.

1. Calculation of Adiabatic Flame Temperature

For an adiabatic process (no heat exchange with the surroundings), the heat balance of the process may be expressed by Equation (61).

$$\sum nH_f^0\text{reactants} = \sum nH_f^0\text{products} + \int_{298}^{TF} nCpdT(\text{products}) \qquad (61)$$

where: T_F = adiabatic flame temperature, K
H_f^0 = heat of formation, calories/mole
C_p = heat capacity of products, calories/mole-K
n = number of moles of reactants or products

The heat of reaction is the heat of formation of products minus the heat of formation of reactants, so upon rewriting Equation (61):

$$-\Delta H\text{reaction} = \int nCpdT(\text{products}) \tag{62}$$

The low-pressure heat capacity of a material is a function of the absolute temperature at which the heat capacity is measured. The temperature dependence of the heat capacity term is expressed in Equation (63).

$$Cp = A + BT + CT^2 + DT^3 \tag{63}$$

where: C_p = heat capacity, calories/mole-K
T = temperature, K

A,B,C,D = heat capacity coefficients,
calories/mole-K, calories/mole-K^2,
calories/mole-K^3, calories/mole-K^4, respectively.

Upon integration of Equation (63), an expression is derived relating the final adiabatic flame temperature to the heats of formation of products and reactants and the heat capacity coefficients of the gaseous combustion products and vaporized propellants.

$$\sum nH_f^0\text{reactants} - \sum nH_f^0\text{products} = -\Delta H\text{reaction} \tag{64}$$

$$-\Delta H\text{reaction} = AT_F + \frac{B}{2}T_F^2 + \frac{C}{3}T_F^3 + \frac{D}{4}T_F^4 + E \tag{65}$$

where: $E = -A(298) - \frac{B}{2}(298)^2 - \frac{C}{3}(298)^3 - \frac{D}{4}(298)^4$
T_F = adiabatic flame temperature, K

The low-pressure heat capacity coefficients for fireball reaction products, as well as the standard free energies of formation for reactants and products, were obtained from a variety of standard reference sources are presented in Table 12. The vapor-phase heat capacity for nitric acid (HNO_3), unsymmetrical dimethylhydrazine (UDMH), and n-dodecane ($C_{12}H_{26}$) were not readily available in the literature, so these values and their corresponding heat capacity coefficients were estimated using Dobratz's Equation (Reference 39). The sensible and latent heats for propellant vaporization are not required in this analysis, since these heats are already included in the heats of formation of the propellant vapors at 298 K. The calculation of the heat of formation of propellant vapors at 298 K has been described previously (Reference 5).

TABLE 12. THERMOCHEMICAL PROPERTIES FOR SOLID AND LIQUID PROPELLANTS AND THEIR COMBUSTION PRODUCTS

SPECIES	ΔH^o_f cal/mole	TEMP RANGE Kelvin	HEAT CAPACITY COEFFICIENTS A cal/mole-K	B cal/mole-K^2	C cal/mole-K^3	D cal/mole-K^4	E cal/mole
NH_4ClO_4(s)	-70690						
HTPB(s)*	-4241						
PBAN(s)†	-3434						
Al(s)	0						
Fe_2O_3(s)	-197000						
O_2(l)	-3124						
O_2	0						
RP-1(l)‡	-6220						
N_2O_4(l)	-4676						
UDMH(l)	12339						
N_2H_4(l)	12054						
N_2	0						
CO_2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
H_2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
H_2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
N_2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
Al_2O_3(l)**	-381150	2315-5000	3.4620E+01	0.0000E+00	0.0000E+00	0.0000E+00	-1.0320E+04
Al_2O_3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
O_2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
NH_3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
CH_4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
C_2H_4	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
NO_2	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
HNO_3	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
NOCl	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
N_2H_4	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
UDMH	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
N_2O_4	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
$C_{12}H_{26}$	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04
Fe_2O_3(s)	-197000	1000-2500	8.0480E+01	-9.1670E-02	6.3250E-05	-1.3760E-08	-2.0440E+04

Notes: * HTPB empirical formula is $CH_{1.622}$
† PBAN empirical formula is $CH_{1.427}O_{.095}N_{.021}$
‡ RP-1 empirical formula is $CH_{1.95}$
**Al_2O_3 liquid selected when combustion cloud >2315 K, melting point of aluminum oxide
ΔH^o_f = heat of formation (calories/mole)
$C_p = A + BT + CT^2 + DT^3$ (calories/mole-K)
Species are gaseous unless otherwise noted by (l) or (s).

B. CALCULATION OF FIREBALL SIZE

Fireball size calculations employing two methods are described in this report. The first method employs an empirical relationship derived from Project Pyro test data (Reference 40) and developed by Gayle and Bransford (Reference 41). For fireballs formed primarily from liquid propellants, the clouds are treated as spheroids. The correlation developed by the researchers is:

$$\text{Diameter} = 8.86 W_b^{0.328} \tag{66}$$

$$\text{Volume} = \frac{1}{6}\pi D^3 = 364.2 W_b^{0.984} \quad ; W_b = \text{Total Propellant Weight, Pounds} \tag{67}$$

Because these empirical relationships were developed for accidents involving liquid propellants, their application to clouds arising from the combustion of solid rocket propellants is not appropriate. For solid rocket propellants, a variable quantity of entrained air, dependent on the exact time and altitude of abort, contributes to the final fireball volume. Equations (66) and (67) do not provide for the entrainment of air into a fireball involving solid rocket propellants. For this case, an approach using the ideal gas law was employed. The equation used to predict the size of combustion cloud resulting from the combustion of solid rocket propellants in which a variable amount of entrained air is added is shown in Equation (68).

$$\text{Diameter} = \sqrt[3]{\frac{6 W_g R T}{\mathcal{M} \pi P}} \tag{68}$$

where: W_g = Total Weight of Combustion Gases*, Pounds

R = Ideal Gas Constant = 0.7302 $\dfrac{ft^3 - atm}{lb - mole°R}$

T = Absolute Temperature, °R

$\mathcal{M}$ = Average Molecular Weight, lb/lb-mole

P = Pressure, atmospheres

π = 3.1416

*Including entrained air and neglecting solid or liquid condensates such as Al_2O_3 and Fe_2O_3

Using representative values for solid combustion clouds of R=0.7302, T = 4725°R, $\mathcal{M}$ =27.29 lb/lb-mole, and P = 1 atmosphere, and assuming a 35% air entrainment ratio (lbs air/lb solids at abort) this relationship reduces to:

$$\text{Diameter} = 6.23 W_g^{0.333} \tag{69}$$

W_g is used in place of W_b to indicate that the total weight includes the weight of the propellants and the weight of entrained air, less the weight of solid or liquid combustion products. This example is taken from the Delta II accident, Test Case 2, lower cloud (See Section V Paragraph E). One can readily see the correlation between Equations (66) and (69). The differences in the empirical formula and the formula derived from the ideal gas law may be ascribed to a variety of factors. The combustion gases are hot and are not likely ideal, thermal radiation effects have been neglected, the pressure inside the fireball cloud is likely less than one atmosphere as the explosion sends combustion gases radially from the center, and the exact quantities of entrained air for both liquid and solid clouds is unknown. Reducing the uncertainties in effective fireball temperatures as well as the exact quantities of entrained air into the propellant clouds during fireball formation would provide a better agreement between the empirical and theoretical correlations of fireball size.

C. ASSUMPTIONS AND CONDITIONS

In formulating source models for the Titan II, Delta II, and Titan IV launch vehicles, certain assumptions regarding the nature and extent of propellant reactions are required. Limitations of available information with respect to these reactions in a launch vehicle explosion are evident and are discussed in Section IV. In particular, the absence of empirical data on the extent of bipropellant reactions during an explosive event, the identification of reaction products (including vaporized propellants), and the degree to which both reactants and products are thermally decomposed in the ensuing fireball require estimates of these properties based on scientific and engineering analyses.

These analyses are based on input from the Project Pyro tests, worked performed by the authors in previous studies, and on data previously unavailable at the time the earlier studies were completed. Because little data exist for the determination of critical fireball parameters, these parameters are assigned a "default" value as well as probable ranges based on an engineering analysis of a typical launch vehicle explosion. A rigorous statistical distribution of the ranges of these input parameters, as well as a Monte Carlo simulation of the effects of these parameters on final fireball results are outside the scope of the current contract. Such a study would, however, be useful in providing a probabilistic range of fireball output data (temperature, size, and chemical composition) instead of a deterministic value.

Specific assumptions used during development of the Titan II, Delta II, and Titan IV chemical source models are documented below:

1. Approximately 23 percent of the original Aerozine-50/nitrogen tetroxide propellant inventory reacts to form the explosive event. This value was determined upon review of Project Pyro heat flux measurements taken from Aerozine-50/nitrogen tetroxide 1,000 pound tests. This analysis is documented in its entirety in Section IV. The range of values expected for this parameter is between 10 and 40 percent.

2. Approximately 44 percent of the original RP-1/liquid oxygen propellant inventory also reacts to form the explosive event. This value was determined upon review of Project Pyro heat flux measurements taken from RP-1/LOX 25,000 pound tests. This analysis is likewise documented in its entirety in Section IV. The range of values expected for this parameter is between 10 and 70 percent.

3. Because the Delta II and Titan IV launch vehicles are fueled by both liquid and solid rocket propellants, two distinct chemical clouds are expected to form: an upper cloud consisting of combustion products of the liquid rocket propellants, and a lower cloud consisting of combustion products of the solid rocket propellants. The lower cloud also contains a considerable degree of entrained air. The development of the two-cloud model in describing launch vehicles accidents involving both liquid and solid rocket propellants was first applied to the Titan 34D launch vehicle (Reference 6).

4. In an on-pad accident, 10 percent of the solid propellants contribute to the formation of the upper fireball cloud. The remaining 90 percent of the solid propellants burn in air on the ground surface.

5. In an in-flight accident, five percent of the solid propellants contributes to the formation of the upper fireball cloud, and the remaining 95 percent burns while entraining air during decent to the ground surface.

6. Approximately 94 percent of the hydrazine is expected to experience thermal monodecomposition to form ammonia, hydrogen and nitrogen. This value is determined by calculating the volume fraction of the fireball which exceeds the thermal decomposition temperature of hydrazine (200°C), and is presented in more detail in Appendix E. Because of the uncertainty in predicting hydrazine monodecomposition reactions in a fireball, this value may range from zero percent to 100 percent.

7. Approximately 70 percent of the UDMH is likewise expected to thermally decompose to form methane and nitrogen. This value is similarly determined by the volume fraction of the fireball which exceeds the reported thermal decomposition temperature of UDMH, 500°C. This calculation is presented in Appendix E. This value is also expected to range between zero percent and 100 percent. The value of this variable is slightly different for the Titan II model (65 percent) and is due to the slightly different thermal environments of the Titan II fireball cloud.

8. Approximately 35 percent of vaporized nitrogen dioxide is expected to thermally decompose to form nitrogen and oxygen gases. This value is determined by the volume fraction of the fireball in excess of thermal decomposition temperature for NO_2, estimated to be 900°C, as reported in Section III. This calculation is presented in Appendix E. This value is also expected to range between zero percent and 100 percent.

9. Approximately 75 percent of RP-1 is expected to thermally decompose by hydrocarbon cracking to form ethylene. Cracking is predominant at temperatures above 500°C. This value is determined by the volume fraction of the fireball which exceeds the reported thermal decomposition temperature of RP-1 and is presented in Appendix E. The expected range for this value is between zero percent and 100 percent.

10. Entrained air in the upper (liquid propellant) cloud is expected to be negligible during fireball growth and stabilization. This assumption is based on heat flux measurements taken from the Project Pyro tests. The exact amount of air entrained is an important parameter because it has substantial impact on the composition and temperature of the fireball cloud, and should be evaluated in further detail, outside the scope of this effort. A provision is therefore made for the incorporation of entrained air into the upper fireball cloud.

11. Entrained air in the lower (solid propellant) cloud is dependent on the time and altitude of abort, and is described by the equations presented in Appendix C.

12. No monatomic hydrogen, monatomic oxygen, and hydroxide radicals are expected at fireball temperatures. These chemicals are recombined to form more thermodynamically stable compounds such as water vapor, diatomic oxygen, and diatomic hydrogen.

13. Hydrogen and oxygen gases resulting from the hypergolic combustion between Aerozine-50 and nitrogen tetroxide are combined to form water vapor.

14. Hydrogen gas generated from the solid rocket propellant is likewise combined with oxygen from the entrained air to form water vapor.

15. Additional afterburning reactions with air are expected to occur <u>after</u> dispersion processes begin. Because this effort characterizes chemicals formed during fireball growth until burnout is achieved, these additional reactions are not included in source modeling. Afterburning reactions should, however, be incorporated in subsequent dispersion models. A description of expected reactions between fireball constituents and air is included in Section III E.

D. ASSIGNMENT OF VARIABLES

The following paragraphs describe the assigned variables and engineering constants used in the development of the Titan II, Delta II and Titan IV source models. These assignments are unified as much as possible for the three launch vehicle systems. Deviances, limitations, or special usages of these variables in the preparation of individual source models are discussed in subsequent sections.

(s) Time of Abort This quantity is determined from flight data, and is the recorded flight time in seconds at which the accident or explosion occurs. The time of abort is used to determine residual amounts of nitrogen tetroxide/Aerozine-50, liquid oxygen/RP-1, or unburned solid rocket propellants available for dispersion or further reaction after consumption of propellants during flight.

(A) Altitude of Abort This quantity, also determined from flight data, is the altitude at which the accident or explosion occurs. This value is used in conjunction with the time of abort to determine the quantity of air entrained by solid propellants as they burn free of the vehicle and fall to the ground surface.

(α) Fraction of Total Liquids in Cloud This quantity is the proportion of liquid propellants which contribute to the cloud being modeled. This variable is not applicable to the Titan II model, and the value is expected to range from 0.0 to 1.0. Selected values for the two applicable models (Delta II and Titan IV) are 1.0 for the upper cloud and 0.0 for the lower cloud. All of the liquid propellants (and their respective reaction products) are contained in the upper fireball cloud.

(β) Fraction of Total Solids in Cloud This quantity is the proportion of solid propellants which contribute to the cloud being modeled. This variable is not applicable to the Titan II model. The value of this variable is expected to range from 0.0 to 1.0. For an on-pad accident involving the Delta II or Titan IV launch vehicle, the values determined by engineering analysis are 0.10 for the upper cloud and 0.90 for the lower cloud. Ten percent of the solid propellants (and their combustion products) are contained in the upper cloud. For an in-flight accident involving these vehicles, the vales are 0.05 for the upper cloud and 0.95 for the lower cloud.

(δ) Solid Propellant Reactivity Ratio This quantity is the ratio of the weight of solid propellants which react during a launch vehicle explosion to the total weight of propellants available on the vehicle. The range of this value is uncertain, however in a Titan 34D accident in April 1986, less than one percent of unburned solid rocket propellant was retrieved. The selected value of this variable for incorporation into the Delta II and Titan IV source models is 1.0.

(δ^*) Solid Propellant Consumption Ratio This quantity is the ratio of unburned solid rocket propellants on board the vehicle at the time of abort to the initial loaded weight of solid rocket propellants. This parameter accounts for the reduction of solid rocket propellants which may contribute to an explosive fireball due to the in-flight consumption of the propellant. This parameter is determined by propellant consumption rates and the time of abort as follows:

$$\text{Delta II:}\quad \delta^* = \frac{232{,}000 - 395 \cdot 6s}{232{,}200} \tag{70}$$

$$\text{Titan IV:}\quad \delta^* = \frac{1{,}182{,}000 - 10{,}764 \cdot s}{1{,}182{,}000} \tag{71}$$

where: s = time of accident, from launch (seconds)

(γ) Liquid Propellant Reactivity Ratio, N_2O_4/A-50 This quantity is the ratio of weight of N_2O_4/A-50 liquid propellants which reacts during a launch vehicle explosion to the total weight of propellants available on the vehicle at the time of accident. This variable is a combined value of the initial explosive involvement and continued burning in the fireball and is slightly dependent on failure mode. The expected range of this value is 0.1 to 0.4, and the selected value corresponding to a command destruct failure is 0.23.

(γ1) Liquid Propellant Reactivity Ratio, LOX/RP-1 This quantity is the ratio of the weight of LOX/RP-1 liquid propellants which react during a Delta II launch vehicle explosion to the total weight of propellants at the time of accident. The expected range of this value is 0.1 to 0.7, and the selected value corresponding to an engineering analysis of a Delta II failure is 0.44. The selected value is independent of failure mode.

(γ*) Liquid Propellant Consumption Ratio, N_2O_4/A-50 This quantity is the ratio of unburned liquid propellants on board the vehicle at the time of accident to the initial loaded weight of liquid propellants. This parameter accounts for the reduction of liquid propellants which contributes to an explosive fireball due to the in-flight consumption of the propellant. For the Titan II vehicle, this parameter is related to the fuel expenditure rate of the Stage I engine as follows:

$$\gamma^* = \frac{312{,}169 - 1{,}651 \cdot s}{312{,}169} \tag{72}$$

where: γ^* = fraction of unburned liquid propellant at time of accident
s = time of accident, from launch (seconds)

For the Delta II and Titan IV vehicles, Aerozine-50 and nitrogen tetroxide propellants are located in the upper vehicle stages and are not ignited below 10,000 feet in altitude. For these two vehicles, a value of 1.00 is assigned, indicated the full inventory of Aerozine-50/nitrogen tetroxide is available at the time of accident. If modeling beyond the 10,000 feet altitude is required for future applications, this value may be changed accordingly.

(γ1*) Liquid Propellant Consumption Ratio, LOX/RP-1 This quantity is the ratio of unburned LOX/RP-1 liquid propellants on board the Delta II vehicle at the time of accident to the initial loaded weights of these propellants. This parameter accounts for the reduction of LOX/RP-1 propellants which may contribute to an explosive fireball due to the in-flight consumption of these propellants. This parameter is determined by the propellant flow rate (consumption rate) and the time of accident and is represented as follows:

$$\gamma 1^* = \frac{212{,}900 - 782.1 \cdot s}{212{,}900} \tag{73}$$

where: s = time of accident, from launch (seconds)

(ζ) Air Entrainment Ratio, Liquids This quantity is the number of moles of air entrained into the fireball cloud per mole of liquid propellant available at the time of accident. The source models for the Titan II, Delta II, and Titan IV assume no air entrainment during fireball growth, based on heat flux data from the Project Pyro tests. This variable is, however, incorporated into source models for use, should subsequent tests or analyses indicate significant air entrainment during fireball growth. This quantity defines additional parameters constrained in the development of the three fireball models as follows:

Titan II:

Total moles air entrained at abort = $2.1551\zeta\gamma^*$ (74)

where:
2.1151 = total normalized gram-moles of liquid propellant available at launch

Total moles oxygen = $(0.21)(2.1551\zeta\gamma^*) = 0.4526\zeta\gamma^*$ (75)

Total moles nitrogen = $(0.79)(2.1551\zeta\gamma^*) = 1.7025\zeta\gamma^*$ (76)

Moles hydrazine combusted with air = $(0.2)(0.5)(0.4526\zeta\gamma^*)$(1 mole Hz/mole O_2)
$= 0.04526\zeta\gamma^*$ (77)

where:
0.2 = 1/5 moles available O_2 combusted with hydrazine
0.5 = 50% of O_2 is contained in Aerozine-50 cloud
$0.4526\zeta\gamma^*$ =total moles O_2 available at abort
(1 mole Hz/mole O_2) = reaction stoichiometry for hydrazine combustion

Moles UDMH combusted with air = $(0.8)(0.5)(0.4526\zeta\gamma^*)$(1 mole UDMH/4 mole O_2)
$= 0.04526\zeta\gamma^*$ (78)

where:
0.8 = 4/5 moles available O_2 combusted with UDMH
0.5 = 50% of O_2 is contained in Aerozine-50 cloud
$0.4526\zeta\gamma^*$ = total moles O_2 available at abort
(1 mole UDMH/4 mole O_2) = reaction stoichiometry for UDMH combustion

Conditional Statements:

IF: moles Hz combusted with air > $0.6522(1-\gamma)\gamma^* + 0.0870\gamma^*$
THEN: moles Hz combusted with air = $0.6522(1-\gamma)\gamma^* + 0.0870\gamma^*$

IF: moles UDMH combusted with air > $0.3478(1-\gamma)\gamma^* + 0.0464\gamma^*$
THEN: moles UDMH combusted with air = $0.3478(1-\gamma)\gamma^* + 0.0464\gamma^*$

Delta II:

Total moles air entrained at abort =
$\zeta[\gamma 1^*(0.3203+0.3346)+\gamma^*(0.0067+0.0051+0.0027)] = \zeta[0.6549\gamma 1^*+0.0145\gamma^*]$ (79)

Total moles oxygen = $0.21\zeta[0.6549\gamma 1^*+0.0145\gamma^*]$ (80)

Total moles nitrogen = $0.79\zeta[0.6549\gamma 1^*+0.0145\gamma^*]$ (81)

Moles hydrazine combusted with air =
$(0.01)(0.5)[0.21\zeta(0.6549\gamma 1^*+0.0145\gamma^*)]$(1 mole Hz/mole O_2)=
$\zeta(0.0006876\gamma 1^*+0.00001523\gamma^*)$ (82)

where:
0.01 = 1% of total available moles oxygen react with hydrazine
0.5 = 50% of O_2 is contained in Aerozine-50 cloud
$0.21\zeta(0.6549\gamma 1^*+0.0145\gamma^*)$ = total moles O_2 available at abort
(1 mole Hz/mole O_2) = reaction stoichiometry for hydrazine combustion

Moles UDMH combusted with air =
$(0.021)(0.5)[0.21\zeta(0.6549\gamma 1^*+0.0145\gamma^*]$(1 mole UDMH/4 mole O_2)=
$\gamma(0.0003610\gamma 1^*+0.00000799\gamma^*)$ (83)

where:
0.021 = 2.1% of total available moles oxygen react with UDMH
0.5 = 50% of O_2 is contained in Aerozine-50 cloud
$0.21\zeta(0.6549\gamma 1^*+0.0145\gamma^*)$ = total moles O_2 available at abort
1 mole UDMH/4 mole O_2 = reaction stoichiometry for UDMH combustion

Moles RP-1 combusted with air =
$(0.969)(0.5)[0.21\zeta(0.6549\gamma 1^*+0.0145\gamma^*]$(1mole RP-1/1.5 mole O_2)=
$\gamma(0.04442\gamma 1^*+0.0009835\gamma^*)$ (84)

where:
0.969 = 96.9% of total available moles oxygen react with RP-1
0.5 = 50% of O2 is contained in Aerozine-50 cloud
$0.21\zeta(0.6549\gamma 1^*+0.0145\gamma^*)$ = total moles O_2 available at abort
1 mole RP-1/1.5 mole O_2 = reaction stoichiometry for RP-1 combustion

Conditional Statements:

IF: moles RP-1 combusted with air > $0.3203(1-\gamma 1)(\gamma 1^*)+0.0143\gamma 1^*$
THEN: moles RP-1 combusted with air = $0.3203(1-\gamma 1)(\gamma 1^*)+0.0143\gamma 1^*$

IF: moles UDMH combusted with air > $0.002272(1-\gamma)(\gamma^*)+0.000434\gamma^*$
THEN: moles UDMH combusted with air = $0.002272(1-\gamma)(\gamma^*)+0.000434\gamma^*$

IF: moles Hz combusted with air > $0.00426(1-\gamma)(\gamma^*)+0.0008156\gamma^*$
THEN: moles Hz combusted with air = $0.00426(1-\gamma)(\gamma^*)+0.0008156\gamma^*$

Titan IV:

Total moles air entrained at abort = $0.2026\zeta\gamma^*$ (85)

Total moles oxygen = $0.21(0.2026\zeta\gamma^*) = 0.0425\zeta\gamma^*$ (86)

Total moles nitrogen = $0.79(0.2026\zeta\gamma^*) = 0.1601\zeta\gamma^*$ (87)

Moles hydrazine combusted with air =
$(0.2)(0.5)(0.0425\zeta\gamma^*)(1 \text{ mole Hz/mole } O_2) = 0.00425\zeta\gamma^*$ (88)

where:
0.2 = 1/5 moles O_2 are combusted with hydrazine
0.5 = 50% of O_2 is contained in Aerozine-50 cloud
$0.0425\zeta\gamma^*$ = total moles O_2 available at abort
(1 mole Hz/mole O_2) = reaction stoichiometry for hydrazine combustion

Moles UDMH combusted with air =
$(0.8)(0.5)(0.0425\zeta\gamma^*)(1 \text{ mole UDMH/4 moles } O_2) = 0.00425\zeta\gamma^*$ (89)

where:
0.8 = 4/5 moles O_2 are combusted with UDMH
0.5 = 50% of O_2 is contained in Aerozine-50 cloud
$0.0425\zeta\gamma^*$ = total moles O_2 available at abort
(1 mole UDMH/4 mole O_2) = reaction stoichiometry for UDMH combustion

Conditional Statements:

IF: moles UDMH combusted with air > $0.0309(1-\gamma)(\gamma^*)+0.0061\gamma^*$
THEN: moles UDMH combusted with air = $0.0309(1-\gamma)(\gamma^*)+0.0061\gamma^*$

IF: moles Hz combusted with air > $0.0579(1-\gamma)(\gamma^*)+0.0115\gamma^*$
THEN: moles Hz combusted with air = $0.0579(1-\gamma)(\gamma^*)+0.0115\gamma^*$

The Fortran 77 code developed for this project (Reference 2) uses a variable, termed the Fraction Excess Air Entrained (FAEE), which for the Titan II and Titan IV models is identical to the Air Entrainment Ratio and has units of moles of air entrained per mole of liquid propellant available at the time of accident. In the development of the Fortran 77 code for the Delta II model, however, the units of this variable are pounds of air entrained per pound of liquid propellant available. The correlation between the Air Entrainment Ratio (ζ) used for the Delta II source model and the Fraction Excess Air Entrained (FAEE) used in the Delta II software encoding is as follows:

$$\mathrm{FAEE} = \zeta \cdot \frac{28.964\left[\gamma 1^{*}(0.6549) + \gamma^{*}(0.0146)\right]}{\gamma 1^{*}(14.9259) + \gamma^{*}(0.94542)} \tag{90}$$

where:
FAEE = Fraction Excess Air Entrained, (lb air/lb liquid propellants at abort)
ζ = Air Entrainment Ratio, (g-moles air/g-moles liquid propellants at abort)
$\gamma 1^{*}$ = Liquid Propellant Consumption Ratio, LOX/RP-1
γ^{*} = Liquid Propellant Consumption Ratio, N_2O_4/A-50

<u>(ε) Fraction Excess Hydrazine Monodecomposed</u> This quantity is the fractional amount of hydrazine thermally decomposed after reacting with nitrogen tetroxide and entrained oxygen (if applicable). Hydrazine may experience thermal decomposition in accordance with:

$$N_2H_4(g) \rightarrow NH_3 + 0.5\ N_2 + 0.5\ H_2 \tag{91}$$

The expected range for this value is 0.0 to 1.0, and the selected value is 0.94 based on thermal gradient analysis of the expected fireball.

<u>(η) Fraction Excess Hydrazine Vaporized or Condensed = 1- ε</u> By mass balance, the remaining hydrazine is vaporized in the cloud, or condensed as the cloud is allowed to cool. The partitioning of the excess hydrazine into the vapor and condensed phases is governed by the equilibrium vapor pressure relationship as a function of temperature, and is reported in a variety of reference sources.

<u>(ξ) Fraction Excess UDMH Thermally Decomposed</u> This quantity is the fractional amount of unsymmetrical dimethylhydrazine thermally decomposed after reacting with nitrogen tetroxide and entrained oxygen (if applicable). UDMH may experience thermal decomposition in accordance with:

$$C_2H_8N_2(g) \rightarrow 2\ CH_4 + N_2 \tag{92}$$

The expected range for this value is 0.0 to 1.0, and the selected value is 0.65 for the Titan II, 0.70 for the Delta II, and 0.70 for the Titan IV vehicles, respectively, based on thermal gradient analyses of the expected fireballs.

(ι) Fraction Excess UDMH Vaporized or Condensed = 1-ξ By mass balance, the remaining UDMH is vaporized in the cloud, or condensed as the cloud is allowed to cool. The partitioning of the excess hydrazine into the vapor and condensed phases is governed by the equilibrium vapor pressure relationship of UDMH as a function of temperature, and is reported in a variety of referenced sources.

(κ) Fraction Excess Nitrogen Tetroxide Converted to NO_2 The dissociation of nitrogen tetroxide into two molecules of nitrogen dioxide is governed by thermodynamic equilibrium, and thus is a function of temperature. Expected range of this variable is between 0.18 and 1.00, with a selected value of 1.00. This selection is based on 18 percent dissociation at 298 K and 88 percent dissociation at 373 K. At expected fireball temperatures, all excess N_2O_4 will be dissociated.

(λ) Fraction Excess Nitrogen Dioxide Thermally Decomposed This quantity represents the fractional quantity of nitrogen dioxide irreversibly thermally decomposed to molecular nitrogen and molecular oxygen. Because the NO_2 is generated from the vapor phase dissociation of N_2O_4, this also represents the fractional quantity of initial N_2O_4 removed by means of this mechanism.

$$N_2O_4 \rightarrow 2NO_2 \rightarrow N_2 + 2O_2 \tag{93}$$

The expected range of this variable is between 0.0 and 0.6, and the selected value is 0.35 based on thermal gradient analysis of the resulting fireball.

(μ) Fraction Excess RP-1 Thermally Decomposed (Cracking) This quantity is the fraction of excess RP-1 thermally decomposed, after reaction with liquid oxygen and entrained oxygen (if applicable), by hydrocarbon cracking to form ethylene C_2H_4.

$$CH_2 \xrightarrow{\Delta} \frac{1}{2} C_2H_4 \tag{94}$$

Cracking is predominant at temperatures above 500°C. The expected range for this value is 0.00 to 1.00, and the selected value is 0.75, based on the thermal gradient analysis of the expected fireball. This variable is only applicable to accidents involving the Delta II launch vehicle.

(υ) Fraction Excess RP-1 Vaporized = 1 - μ By mass balance, the remaining RP-1 is vaporized in the cloud, or condensed as the cloud is allowed to cool. The chemical specified in the model as vaporized or condensed RP-1 is normal dodecane, $C_{12}H_{26}$, although in reality the vapors or condensates are a complex mixture of aliphatic straight chain and cyclic hydrocarbons. The partitioning of excess RP-1 into the vapor and condensed phases is a function of the equilibrium composition of the mixture. This variable is also only applicable to accidents involving the Delta II launch vehicle.

(π) Fraction of Solids which Entrain Air In accidents involving solid rocket propellants (Delta II and Titan IV launch vehicles), solids in the upper cloud are mixed with liquid propellants and their combustion products, and negligible air entrainment of the solid propellant occurs. Conversely, solids in the lower cloud entrain air as they fall to the ground surface. The value of this variable is therefore established as 0.00 for the upper cloud and 1.00 for the lower cloud. The use of these two values for this dummy variable aids in the construction of the mathematical model.

(ρ) Air Entrainment Ratio In accidents involving solid rocket propellants (Delta II and Titan IV launch vehicles), this variable is defined as the number of moles of air entrained per mole ammonium perchlorate (AP) in the solid propellant. This value is determined by analysis, and uses the total weight of air entrained in the solid propellants as a function of abort time and altitude, as described in Appendix C. The following equations determine the air entrainment ratio for the Delta II launch vehicle and Titan IV launch vehicle, respectively.

Delta II:

$$\rho = \frac{W_a \times \dfrac{1\ \text{lb} - \text{mole air}}{28.85\ \text{lb}}}{0.946 \times [232{,}200 - 395(s)(6)\ \text{lb GEM}] \times \dfrac{0.696\ \text{lb AP}}{\text{lb GEM}} \times \dfrac{\text{lb} - \text{mole AP}}{117.46\ \text{lb AP}}} \qquad (95)$$

where:

ρ = Air Entrainment Ratio, moles of air/mole ammonium perchlorate
W_a = Weight of Air Entrained into Burning Solids, pounds (See Appendix C)
s = Time of abort, from launch (seconds)

For a weight of air of 1.0983×10^5 pounds, corresponding to an on-pad abort of a Delta II vehicle, the air entrainment ratio calculated is 2.9248. For activation of the command destruct system at 5000 feet altitude, 3.0694×10^5 pounds air are entrained, and the air entrainment ratio is 10.928.

Titan IV:

$$\rho = \frac{W_a \times \dfrac{1\ \text{lb} - \text{mole air}}{28.85\ \text{lb}}}{\beta \times [1{,}182{,}000 - 10{,}764 \times s\ \ \text{lb SRM}] \times \dfrac{0.6751\ \text{lb AP}}{\text{lb SRM}} \times \dfrac{\text{lb} - \text{mole AP}}{117.489\ \text{lb AP}}} \qquad (96)$$

where:

ρ = Air Entrainment Ratio, moles of air/moles ammonium perchlorate
W_a = Weight of Air Entrained into Burning Solids, pounds (See Appendix C)
β = Fraction total solids in lower cloud
= 0.90 pad abort, 0.95 in-flight abort
s = Time of Abort, from launch (seconds)

For a weight of air of 5.319×10^5 pounds, corresponding to an on-pad abort of a Titan IV vehicle, the air entrainment ratio is 3.0162. For activation of the command destruct system at 25 seconds and 5000 feet altitude, 7.32629×10^5 pounds air are entrained, and the air entrainment ratio is 5.0959.

(σ) HCl Reactivity: $\alpha = 0, \sigma = 0; \alpha > 0, \sigma = 1$ The incorporation of this variable allows for interaction of hydrogen chloride (HCl) with nitrogen tetroxide (N_2O_4) to produce nitric acid (HNO_3) and nitrosyl chloride (NOCl) in the upper cloud. Fifty percent of available HCl is expected to react in this manner.

E. SOURCE MODEL, TITAN II

1. Propellant Loading.

The nominal propellant loading and consumption rates for the Aerozine-50 and nitrogen tetroxide liquid rocket propellants used on the Titan II missile system are included in Table 13. These data are taken from References 42 and 43.

TABLE 13. TITAN II PROPELLANT LOADING AND CONSUMPTION RATES.

Parameter	Value	Units	Reference
Loaded Weight, Aerozine-50	104,609	pounds	42
Loaded Weight, Nitrogen Tetroxide	207,560	pounds	42
Stage I Burn-Out Altitude	250,000	feet	43
Nitrogen Tetroxide Flow Rate, Stage I Engine	1086.6	pounds per second	43
Nitrogen Tetroxide Flow Rate, Stage I Gas Generator	1.7	pounds per second	43
Aerozine-50 Flow Rate, Stage I Engine	543.4	pounds per second	43
Aerozine-50 Flow Rate, Stage I Gas Generator	20.05	pounds per second	43
Stage I Rated Duration	165	seconds	43
Nitrogen Tetroxide Flow Rate, Stage II Engine	204	pounds per second	43
Aerozine-50 Flow Rate, Stage II Engine	113	pounds per second	43
Stage II Rated Duration	185	seconds	43

Molar coefficients of reactants (hydrazine, unsymmetrical dimethylhydrazine, and nitrogen tetroxide) used for modeling are included in Table 14.

TABLE 14. MOLAR COEFFICIENTS USED FOR TITAN II MODELING.

Reactant	Formula	Weight, lbs.	Molecular Weight (gram/g-mole)	actual g-moles	normalized g-moles
Nitrogen Tetroxide	N_2O_4	207,560	92.016	1023160	1.0217
Hydrazine	N_2H_4	52,304.5	32.045	740359	0.7392
UDMH	$C_2H_8N_2$	52,304.5	60.102	394742	0.3942

Notes:
1. Normalized gram-moles are based on 1.0217 gram moles nitrogen tetroxide reacting stoichiometrically.
2. Scaling Factor = actual g-moles N_2O_4/normalized g-moles N_2O_4 = 1.0014×10^6
3. Hydrazine amount includes 46146 pounds hydrazine (0.6522 normalized g-moles) reacting stoichiometrically plus 6158 pounds hydrazine (0.0870 normalized g-moles) in excess.
4. UDMH amount includes 46146 pounds UDMH (0.3478 normalized g-moles) reacting stoichiometrically plus 6158 pounds UDMH (0.0464 normalized g-moles) in excess.

2. Propellant Combustion Reaction.

The hypergolic combustion reaction used for modeling Titan II launch vehicle accidents is shown in Equation (97). This equation is formulated by modifying the complete combustion reaction determined by standard rocket exhaust equilibrium programs (Equation 2) and neglecting the formation of high energy chemicals, such as monatomic hydrogen, monatomic oxygen, and hydroxide radical. Predicted amounts of these energetic chemicals were converted to water vapor, oxygen gas, and hydrogen gas to provide the proper mass balance. High energy compounds are not used in modeling launch vehicle accidents because conversion of these chemicals to more stable compounds occurs upon cooling and dispersion of the fireball cloud. This conversion process releases heat.

$$0.6522\ N_2H_4 + 0.3478\ C_2H_8N_2 + 1.0217\ N_2O_4 \rightarrow 2.6962\ H_2O + 1.9823\ N_2 + 0.3149\ CO_2 + 0.3808\ CO + 0.0761\ NO + 0.1488\ O_2 \quad (97)$$

3. Mathematical Formulation of the Titan II Chemical Source Model

The equations used to determine reactant and product compositions in an accident involving the Titan II missile system are presented in Table 15. These equations incorporate the use of eleven variables, which are established by the specific accident conditions and employ the results of specific analyses described within this report. The stoichiometry of the reactants is taken from the normalized molar loading of these propellants as specified in Table 14. The numerical coefficients are modified by one or more of the eleven variables (fireball parameters) to determine the actual contribution of the individual reactant to the explosive event. For example, the quantity of UDMH which is expected to vaporize under accident conditions is equal to the product of several fractional terms, after burning with residual entrained air is complete. These terms include the fraction of UDMH vaporized (ι), the amount of UDMH remaining after combustion during flight $(0.3478+0.0464)(\gamma^*)$, the amount of UDMH involved in the explosive event with N_2O_4 $(0.3478)(\gamma)(\gamma^*)$, and the amount of UDMH combusted with entrained air $(0.04526\zeta\gamma^*)$.

The amount of UDMH combusted with entrained air cannot exceed the total amount of residual UDMH, therefore a conditional statement is also made:

a_5 = No. moles UDMH (l) combusted in air = $0.04526\zeta\gamma^*$

IF $\quad a_5 > 0.3478(1-\gamma)\gamma^* + 0.0464\gamma^*$;

THEN $\quad a_5 = 0.3478(1-\gamma)\gamma^* + 0.0464\gamma^*$

Reactant coefficient a_5 is the molar quantity of UDMH (liquid) combusted in air. The quantity of UDMH vaporized may therefore be expressed mathematically as:

a_7 = No. moles UDMH vaporized = $\iota[(0.3478+0.0464)\gamma^*-0.3478\gamma\gamma^*-a_5]$

and upon collection of terms:

a_7 = No. moles UDMH vaporized = $\iota[(0.3478)(1-\gamma)\gamma^*+.0464\gamma^*-a_5]$

Reactant coefficient a_7 is the molar quantity of reactant UDMH liquid vaporized during the course of the explosive event. Numerical coefficients for chemical reactants and products for the Titan II missile system are presented in Table 15.

TABLE 15. THERMOCHEMICAL MODEL, TITAN II.

VARIABLE	DEFINITION	UNITS
s	Time of Abort (from launch)	seconds
A	Altitude at Abort	feet
γ	Liquid Propellant Reactivity Ratio	moles liquid propellant reacted/total moles at abort
γ^*	Liquid Propellant Consumption Ratio	moles liquid propellant at abort/total moles loaded
ζ	Air Entrainment Ratio Liquid	moles air entrained/total moles liquid at abort
ε	Fraction Excess Hydrazine Monodecomposed (after air burning)	moles hydrazine decomposed/total moles hydrazine available
η	Fraction Excess Hydrazine Vaporized or Condensed	moles hydrazine vaporized/total moles hydrazine available
ξ	Fraction Excess UDMH Thermally Decomposed (after air burning)	moles UDMH decomposed/total moles UDMH available
ι	Fraction Excess UDMH Vaporized or Condensed	moles UDMH vaporized/total moles UDMH available
κ	Fraction Excess Nitrogen Tetroxide Converted to NO_2	moles N_2O_4 converted to 2 moles NO_2/total moles N_2O_4 available
λ	Fraction Excess NO_2 Thermally Decomposed	moles NO_2 converted to 0.5 moles N_2 and 1.0 moles O_2/total moles NO_2 available
REACTANT COEFFICIENT	**DEFINITION**	**VALUE**
a1	No. moles N_2O_4(l) reacted	$1.0217\gamma\gamma^*$
a2	No. moles N_2O_4(g) decomposed to N_2 + 2 O_2	$\lambda[1.0217(1-\gamma)\gamma^*]$
a3	No. moles N_2O_4 vaporized to $2NO_2$	$(1-\lambda)[1.0217(1-\gamma)\gamma^*]$
a4	No. moles UDMH(l) reacted	$0.3478\gamma\gamma^*$
a5	No. moles UDMH(l) combusted in air IF: $a5 > 0.3478(1-\gamma)(\gamma^*) + 0.0464\gamma^*$; THEN $a5 = 0.3478(1-\gamma)(\gamma^*) + 0.0464\gamma^*$	$0.04526\zeta\gamma^*$
a6	No. moles UDMH (l) thermally decomposed	$\xi(0.3478(1-\gamma)(\gamma^*)+0.0464\gamma^*-a5]$
a7	No. moles UDMH (l) vaporized	$\iota[(0.3478)(1-\gamma)(\gamma^*)+0.0464\gamma^*-a5]$
a8	No. moles N_2H_4(l) reacted	$0.6522\gamma\gamma^*$
a9	No. moles N_2H_4(l) combusted in air IF: $a9>0.6522(1-\gamma)(\gamma^*)+0.0870\gamma^*$; THEN: $a9 = 0.6522(1-\gamma)(\gamma^*)+0.0870\gamma^*$	$0.04526\zeta\gamma^*$
a10	No. moles N_2H_4(l) thermally decomposed	$\varepsilon[0.6522(1-\gamma)(\gamma^*)+0.0870\gamma^*-a9]$
a11	No. moles N_2H_4(l) vaporized	$\eta[0.6522(1-\gamma)(\gamma^*)+0.0870\gamma^*-a9]$
a12	No. moles O_2 entrained in liquid cloud	$0.4526\zeta\gamma^*$
a13	No. moles N_2 entrained in liquid cloud	$1.7025\zeta\gamma^*$
	OTHER USEFUL PARAMETER DEFINITIONS	**VALUE**
	No. moles N_2O_4 consumed in flight	$1.0217(1-\gamma^*)$
	No. moles N_2H_4 consumed in flight	$0.6522(1-\gamma^*)+0.0870(1-\gamma^*)$
	No. moles UDMH consumed in flight	$0.3478(1-\gamma^*)+0.0464(1-\gamma^*)$

TABLE 15. THERMOCHEMICAL MODEL, TITAN II (CONTINUED).

PRODUCT COEFFICIENT	DEFINITION	VALUE
b1	No. moles CO_2 formed by reaction	a1(0.3082)
b2	No. moles CO_2 formed by UDMH-air burn	a5(2.000)
b3	No. moles CO formed by reaction	a1(0.3727)
b4	No. moles H_2O formed by reaction	a1(2.6389)
b5	No. moles H_2O formed by N2H4-air burn	a9(2.000)
b6	No. moles H_2O formed by UDMH air-burn	a5(4.000)
b7	No. moles H_2 formed by N_2H_4 monodecomposition	a10(0.5000)
b8	No. moles N_2 formed by reaction	a1(1.9402)
b9	No. moles N_2 formed by N_2H_4 monodecomposition	a10(0.5000)
b10	No. moles N_2 formed by N_2H_4-air burn	a9(1.000)
b11	No. moles N_2 formed by UDMH decomposition	a6(1.000)
b12	No. moles N_2 formed by UDMH-air burn	a5(1.000)
b13	No. moles N_2 formed by N_2O_4 decomposition	a2(1.000)
b14	No. moles N_2 entrained in liquid cloud	a13
b15	No. moles NO formed by reaction	a1(0.0745)
b16	No. moles O_2 formed by reaction	a1(0.1456)
b17	No. moles O_2 entrained in liquid cloud	a12-4a5-a9
b18	No. moles O_2 formed by N_2O_4 monodecomposition	a2(2.000)
b19	No. moles NH_3 formed by N_2H_4 monodecomposition	a10(1.000)
b20	No. moles N_2H_4 vaporized	a11
b21	No. moles CH_4 formed by UDMH thermal decomposition	a6(2.000)
b22	No. moles UDMH vaporized	a7
b23	No. moles N_2O_4 vaporized	a3(1-κ)
b24	No. moles NO_2 formed from N_2O_4 vapor	a3(κ)(2.000)

TABLE 15. THERMOCHEMICAL MODEL, TITAN II (CONCLUDED).

SUMMARY	VALUE
REACTANTS	
moles N_2O_4 reacted, decomposed, or vaporized	a1+a2+a3
moles UDMH reacted, combusted, decomposed, or vaporized	a4+a5+a6+a7
moles hydrazine reacted, combusted,decomposed,or vaporized	a8+a9+a10+a11
moles O_2 reacted or entrained	a12
moles N_2 entrained	a13
PRODUCTS	
moles CO_2 formed	b1+b2
moles CO formed	b3
moles H_2O formed	b4+b5+b6
moles H_2 formed	b7
moles N_2 formed	b8+b9+b10+b11+b12+b13+b14
moles NO formed	b15
moles O_2 formed	b16+b17+b18
moles NH_3 formed	b19
moles N_2H_4 vaporized	b20
moles CH_4 formed	b21
moles UDMH vaporized	b22
moles N_2O_4 vaporized	b23
moles NO_2 formed	b24

Equations used to determine fireball parameters for an accident involving the Titan II, taken from data in Table 15 and thermodynamic data reported in Table 12, are as follows:

Composition (g – mole) – determined from model

$$\text{Mole\%} = \frac{\text{g} - \text{mole chemical}}{\text{total moles}} \times 100 \tag{98}$$

$$\text{Mass, lb} = \frac{\text{g} - \text{mole chemical} \times \text{SF} \times \mathcal{M}}{453.59\ \text{g}/\text{lb}} \tag{99}$$

$\mathcal{M}$ = Molecular Weight, grams/gram mole
SF = Scaling Factor = 1.00143 x 10^6 (Titan II model)

Adiabatic Flame Temperature

$$0 = \Delta\text{Hrxn} + \text{AT}_\text{F} + \frac{\text{B}}{2}\text{T}_\text{F}^2 + \frac{\text{C}}{3}\text{T}_\text{F}^3 + \frac{\text{D}}{4}\text{T}_\text{F}^4 + \text{E} \tag{100}$$

T_F = Adiabatic Flame Temperature: determined by iteration

$$\text{Average Molecular Weight} = \frac{\sum(\text{moles} \times \mathcal{M})}{\sum \text{moles}} \tag{101}$$

Fireball Size:

$$\text{Diameter} = 8.86\,\text{Wb}^{0.328} \tag{102}$$

$$\text{Volume} = \frac{4}{3}\pi r^3$$

$$\text{Total Heat Release} = \frac{\Delta\text{Hrxn}}{1.0217\ \text{g} - \text{mole N2O4}} \times \text{SF} \tag{103}$$

4. Default Values and Suggested Ranges.

Table 16 shows the suggested values of the eleven input variables for a Titan II on-pad abort (Case 1), a set of values for a hypothetical in-flight abort incorporating air entrainment (Case 2), and the expected ranges of these variables for all accident conditions. In the absence of other derived data, the variable values in Case 1 are considered the nominal default values for atmospheric dispersion modeling.

TABLE 16. TEST CASE VALUES, TITAN II MODEL.

Variable	Expected Range	Test Case 1 On-Pad Abort Confined by Ground Surface 0 Air Entrainment	Test Case 2 Abort at 5000 Feet Altitude Command Destruct 0.5 Moles Air/Mole Liquids
s	0-60	0.00	20
A	0-10000	0.00	5000
γ	0.10-0.40	0.23	0.23
γ^*	0.68-1.00	1.00	0.89
ζ	0.00-3.00	0.00	0.50
ε	0.00-1.00	0.94	0.94
η	0.00-1.00	0.06	0.06
ξ	0.00-1.00	0.65	0.65
ι	0.00-1.00	0.35	0.35
κ	0.18-1.00	1.00	1.00
λ	0.00-1.00	0.35	0.35

5. Results

Fireball data for the Titan II test cases identified in Table 16 are presented in Tables 17 and 18, respectively. These data include chemical composition, fireball size, total heat released, and adiabatic flame temperature. Computer spreadsheets showing the calculations for these two test cases are contained in Appendix F.

TABLE 17. SOURCE STRENGTH SUMMARY - TITAN II LAUNCH VEHICLE, TEST CASE 1.

Abort Condition: On-Pad Accident; Confined by Ground Surface (CBGS); 0 Air Entrainment		
Propellant Loading:	Aerozine-50	104,609 lbs
	Nitrogen Tetroxide	207,560 lbs
Constituent	Mole %	Mass, lbs
<u>Reactants</u>		
$N_2O_4(l)$	47.41	207,560
$C_2H_8N_2(l)$	18.29	52,307
$N_2H_4(l)$	34.30	52,297
TOTAL	100.00	312,164
<u>Products</u>		
$CO_2(g)$	1.45	7,037
$CO(g)$	1.75	5,416
$H_2O(g)$	12.40	24,664
$H_2(g)$	5.54	1,233
$N_2(g)$	24.24	74,985
$NO(g)$	0.35	1,160
$O_2(g)$	11.69	41,322
$NH_3(g)$	11.07	20,824
$CH_4(g)$	8.17	14,468
$NO_2(g)$	20.45	103,879
<u>Vaporized Propellants</u>		
$C_2H_8N_2(g)$	2.20	14,592
$N_2H_4(g)$	0.71	2,501
$N_2O_4(g)$	0.00	0
TOTAL	100.02	312,081
Adiabatic Flame Temperature		1342 K
Average Molecular Weight		28.26 grams/g-mole
Fireball Size		
Diameter		562 feet
Volume		9.285×10^7 cubic feet
Total Heat Released		-5.587×10^{10} calories

TABLE 18. SOURCE STRENGTH SUMMARY - TITAN II LAUNCH VEHICLE, TEST CASE 2.

Abort Condition: In-Flight Accident; Command Destruct; 0.5 Air Entrainment Ratio		
Propellant Loading:	Aerozine-50	104,609 lbs
	Nitrogen Tetroxide	207,560 lbs
Constituent	Mole %	Mass, lbs
Consumed in Flight		
N_2O_4(l)		22,834
$C_2H_8N_2$(l)		5,759
N_2H_4(l)		5,752
Reactants		
N_2O_4(l)	31.61	184,728
$C_2H_8N_2$(l)	12.19	46,554
N_2H_4(l)	22.87	46,545
O_2(g)	7.00	14,229
N_2(g)	26.33	46,856
TOTAL	100.00	338,912
Products		
CO_2(g)	1.93	10,177
CO(g)	1.44	4,820
H_2O(g)	12.40	26,757
H_2(g)	4.37	1,055
N_2(g)	34.17	114,689
NO(g)	0.29	1,032
O_2(g)	11.45	43,891
NH_3(g)	8.74	17,821
CH_4(g)	6.22	11,949
NO_2(g)	16.77	92,453
Vaporized Propellants		
$C_2H_8N_2$(g)	1.67	12,052
N_2H_4(g)	0.56	2,140
N_2O_4(g)	0.00	0
TOTAL	100.01	338,836
Adiabatic Flame Temperature	1384 K	
Average Molecular Weight	28.28 grams/g-mole	
Fireball Size		
Diameter	541 feet	
Volume	8.279×10^7 cubic feet	
Total Heat Released	-6.001×10^{10} calories	

F. SOURCE MODEL, DELTA II

1. Propellant Loading

The nominal propellant loading and consumption rates for the liquid rocket propellants (liquid oxygen and RP-1) and the graphite epoxy motor (GEM) solid rocket propellant on the Delta II 7925 launch vehicle are shown in Table 19. Data for this table were taken from Reference 44 and from the McDonnell Douglas Corporation[9].

TABLE 19. DELTA II 7925 PROPELLANT LOADING AND CONSUMPTION RATES.

Stage	Parameter	Value	Units
Booster	Loaded Weight, Liquid Oxygen	146,200	pounds
	Loaded Weight, RP-1	66,700	pounds
	Engine	Rocketdyne RS2701C	
	Mixture Ratio	2.245:1	pounds LOX/pound RP-1
	Liquid Oxygen Flow Rate Main Engine	537.14	pounds per second
	Liquid Oxygen Flow Rate Gas Generator	4.86	pounds per second
	RP-1 Flow Rate Main Engine	225.49	pounds per second
	RP-1 Flow Rate Gas Generator	14.61	pounds per second
	Rated Engine Duration	227 242	seconds, nominal seconds, maximum
2nd Stage	Loaded Weight, Nitrogen Tetroxide	8,759	pounds
	Loaded Weight, Aerozine-50	4,640	pounds
3rd Stage†	Loaded Weight, TP-H-3340 Solid Propellant	4,450	pounds
Solids	Loaded Weight, GEMS QBJ-29	9 motors @ 25,800 pounds/motor	pounds

Notes: † Not included in source strength modeling; upper stage.

Molar coefficients of reactants (LOX, RP-1, hydrazine, unsymmetrical dimethylhydrazine, nitrogen tetroxide, ammonium perchlorate, aluminum, and HTPB) are included in Table 20.

[9]Data Taken from Rocketdyne RS2701A engine which is similar, but not identical to RS2701C engine. Delta II Vehicle and Mission Description. McDonnell Douglas Corporation. September, 1993.

TABLE 20. MOLAR COEFFICIENTS USED FOR DELTA II MODELING.

Reactant	Formula	Weight, lbs.	Molecular Weight (g/g-mole)	actual g-mole	normalized g-moles
Ammonium Perchlorate	NH_4ClO_4	161,611	117.489	623,932	0.0965
HTPB	$CH_{1.622}$	26,099	13.646	867,525	0.1341
Aluminum	Al	44,490	26.982	747,914	0.1156
Liquid Oxygen	O_2	146,200	31.999	2,072,404	0.3203
RP-1	$CH_{1.95}$	66,700	13.976	2,164,743	0.3346
Nitrogen Tetroxide	N_2O_4	8,759	92.016	43,177	0.0067
Hydrazine	N_2H_4	2,320	32.045	32,839	0.005076
UDMH	$C_2H_8N_2$	2,320	60.102	17,509	0.002706

Notes:
1. Normalized g-moles are determined by dividing actual g-moles by the total amount of all propellants reacting stoichiometrically, exclusive of fuel-rich loadings of RP-1, hydrazine, and UDMH (6.4702×10^6 gram-moles). This latter value is also the scaling factor.
2. RP-1 amount includes 63,855 pounds RP-1 reacting stoichiometrically (0.3203 normalized g-moles) plus 2,845 pounds RP-1 (0.0143 normalized g-moles) excess for fuel-rich propellant loading.
3. Hydrazine amount includes 1,947 pounds hydrazine reacting stoichiometrically (0.00426 normalized g-moles) plus 373 pounds hydrazine (0.0008156 normalized g-moles) excess for fuel-rich propellant loading.
4. UDMH amount includes 1,947 pounds UDMH reacting stoichiometrically (0.002272 normalized g-moles) plus 373 pounds UDMH (0.000434 normalized g-moles) excess for fuel-rich propellant loading.

2. Propellant Combustion Reactions

Propellant combustion reactions used in the development of the Delta II Source Model are presented in the following equations. The equations used were simplified reactions in which free radicals were recombined to form more stable chemical compounds, and residual hydrogen and oxygen were reacted to form water vapor.

a. Aerozine-50 and Nitrogen Tetroxide

$$0.6522\ N_2H_4 + 0.3478\ C_2H_8N_2 + 1.0217\ N_2O_4 \rightarrow 2.6962\ H_2O + 1.9823\ N_2 + 0.3149\ CO_2 + 0.3808\ CO + 0.0761\ NO + 0.1488\ O_2 \quad (104)$$

$T_F = 3763$ K
$\Delta H_{rxn} = -2.01 \times 10^5$ calories

b. RP-1 and Liquid Oxygen

$$1.0000\ CH_{1.95} + 1.0000\ O_2\ (l) \rightarrow 0.3333\ CO_2 + 0.3333\ H_2 + 0.6667\ CO + 0.6667\ H_2O \quad (105)$$

$T_F = 4017$ K
$\Delta H_{rxn} = -8.025 \times 10^4$ calories

c. GEM Solids

$$1.0000\ NH_4ClO_4 + 1.3904\ CH_{1.622} + 1.1987\ Al \rightarrow 0.0808\ CO_2 + 1.2974\ CO + 0.7803\ H_2O + 1.8315\ H_2 + 0.4978\ N_2 + 0.9679\ HCl + 0.5739\ Al_2O_3\ (l) \qquad (106)$$

$T_F = 3916$ K
$\Delta H_{rxn} = -2.506 \times 10^5$ calories

d. RP-1 and Air

$$CH_2 + \frac{3}{2} O_2 \rightarrow CO_2 + H_2O \qquad (107)$$

$T_F = 5330$ K
$\Delta H_{rxn} = -1.46 \times 10^5$ calories

e. RP-1 Thermal Decomposition

$$CH_2 \xrightarrow{\Delta} \frac{1}{2} C_2H_4 \qquad (108)$$

T_F = undefined (endothermic process)
$\Delta H_{rxn} = +1.25 \times 10^4$ calories

3. Mathematical Formulation of the Delta II Chemical Source Model

The equations used to determine reactant and product compositions involving the Delta II launch vehicle system are presented in Table 21. The equations are comprised of 22 variables developed for the Delta II model, the values of which are determined by the specific accident conditions and assumptions used. The stoichiometry of the reactants is taken from the normalized molar loading presented in Table 20. Reactants and products are modified by one or more of the 22 variables to determine their contributions to the explosive event. Establishment of a mass balance within the accuracy of the source model is verified. In the case of the Delta II vehicle, two combustion clouds are generated by the model: an upper cloud consisting of products of the liquid propellant reactions; and a lower cloud consisting of the combustion products of the solid propellants and containing entrained air.

TABLE 21. THERMOCHEMICAL MODEL, DELTA II.

VARIABLE	DEFINITION	UNITS
s	Time of Abort (from launch)	seconds
A	Altitude at Abort	feet
α	Fraction Total Liquids in Cloud	moles liquid propellant in cloud/total moles of liquid propellant in all clouds
β	Fraction Total Solids in Cloud	moles solid propellant in cloud/total moles of solid propellant in all clouds
δ	Solid Propellant Reactivity Ratio	moles solid propellant reacted/total moles at abort
δ^*	Solid Propellant Consumption Ratio	moles solid propellant at abort/total moles loaded
γ	Liquid Propellant Reactivity Ratio, N_2O_4/A-50	moles N_2O_4/A-50 reacted/total moles at abort
γ^*	Liquid Propellant Consumption Ratio, N_2O_4/A-50	moles N_2O_4/A-50 at abort/total moles loaded
$\gamma 1$	Liquid Propellant Reactivity Ratio, LOX/RP-1	moles LOX/RP-1 reacted/total moles at abort
$\gamma 1^*$	Liquid Propellant Consumption Ratio, LOX/RP-1	moles LOX/RP-1 at abort/total moles loaded
ζ	Air Entrainment Ratio, Liquids	moles air entrained/total moles liquids at abort
ε	Fraction Excess Hydrazine Monodecomposed (after air burning)	moles hydrazine decomposed/total moles hydrazine available
η	Fraction Excess Hydrazine Vaporized or Condensed	moles hydrazine vaporized/total moles hydrazine available
ξ	Fraction Excess UDMH Thermally Decomposed (after air burning)	moles UDMH decomposed/total moles UDMH available
ι	Fraction Excess UDMH Vaporized or Condensed	moles UDMH vaporized/total moles UDMH available
κ	Fraction Excess Nitrogen Tetroxide Converted to NO_2	moles N_2O_4 converted to 2 moles NO_2/total moles N_2O_4 available
λ	Fraction Excess NO_2 Thermally Decomposed	moles NO_2 converted to 0.5 moles N_2 and 1.0 mole O_2/total moles NO_2 available
μ	Fraction Excess RP-1 Thermally Decomposed After Air Burning (Cracking)	moles RP-1 decomposed/total moles RP-1 available
υ	Fraction Excess RP-1 Vaporized or Condensed	moles RP-1 vaporized (as $C_{12}H_{26}$)/total moles RP-1 available
π	Fraction of Solids which Entrain Air	moles of solids entraining air/total moles solids available
ρ	Air Entrainment Ratio, Solids	moles of air entrained/moles ammonium perchlorate available
σ	HCl reactivity	"dummy variable": $\alpha=0,\sigma=0$; $\alpha>0,\sigma=1$
REACTANT COEFFICIENT	**DEFINITION**	**VALUE**
a1	No. moles $NH_4ClO_4(s)$ reacted	$0.0965\beta\delta\delta^*$
a2	No. moles $CH_{1.622}(s)$ reacted	$0.1341\beta\delta\delta^*$
a3	No. moles Al(s) reacted	$0.1156\beta\delta\delta^*$
a4	No. moles O_2 entrained in liquid	$0.21\zeta\alpha[0.6549\gamma 1^*+0.0145\gamma^*]$
a5	No. moles O_2 entrained in solid	$0.21(a1)\rho\pi$
a6	No. moles N_2 entrained in liquid	$0.79\zeta\alpha[0.6549\gamma 1^*+0.0145\gamma^*]$
a7	No. moles N_2 entrained in solid	$0.79(a1)\rho\pi$
a8	No. moles RP-1 reacted	$0.3203\gamma 1\gamma 1^*\alpha$
a9	No. moles RP-1 combusted in air IF: $a9>0.3203(1-\gamma 1)(\gamma 1^*)+0.0143\gamma 1^*$; THEN $a9=0.3203(1-\gamma 1)(\gamma 1^*)+0.0143\gamma 1^*$	$\zeta\alpha[0.04442\gamma 1^*+0.0009835\gamma^*]$
a10	No. moles RP-1 thermally decomposed	$\mu[0.3203(1-\gamma 1)(\gamma 1^*)\alpha+0.0143\gamma 1^*\alpha-a9]$
a11	No. moles RP-1 vaporized	$\upsilon[0.3203(1-\gamma 1)(\gamma 1^*)\alpha+0.0143\gamma 1^*\alpha-a9]$
a12	No. moles $N_2O_4(l)$ reacted	$0.0067\gamma\gamma^*\alpha$

TABLE 21. THERMOCHEMICAL MODEL, DELTA II (CONTINUED).

VARIABLE	DEFINITION	UNITS
a13	No. moles N_2O_4(g) reacted with HCl	$\sigma(0.5000)(a1)$
a14	No. moles N_2O_4(g) decomposed to N_2 + 2 O_2	$\lambda[0.0067(1-\gamma)\gamma^*\alpha-\sigma(0.5000)a1]$
a15	No. moles N_2O_4 vaporized to $2NO_2$	$(1-\lambda)[0.0067(1-\gamma)\gamma^*\alpha-\sigma(0.5000)a1]$
a16	No. moles UDMH(l) reacted	$0.002272\gamma\gamma^*\alpha$
a17	No. moles UDMH(l) combusted in air IF: $a17 > 0.002272(1-\gamma)(\gamma^*) +0.000434\gamma^*$; THEN: $a17 = 0.002272(1-\gamma)(\gamma^*) +0.000434\gamma^*$	$\zeta[0.0003610\gamma 1^*+0.00000799\gamma^*]\alpha$
a18	No. moles UDMH (l) thermally decomposed	$\xi[0.002272(1-\gamma)(\gamma^*)\alpha+0.000434\gamma^*\alpha\text{-a}17]$
a19	No. moles UDMH (l) vaporized	$\iota[0.002272(1-\gamma)(\gamma^*)\alpha+0.000434\gamma^*\alpha\text{-a}17]$
a20	No. moles N_2H_4(l) reacted	$0.00426\gamma\gamma^*\alpha$
a21	No. moles N_2H_4(l) combusted in air IF: $a21>0.00426(1-\gamma)(\gamma^*) +0.0008156\gamma^*$; THEN: $a21 = 0.00426(1-\gamma)(\gamma^*) +0.0008156\gamma^*$	$\zeta[0.0006876\gamma 1^*+0.00001523\gamma^*]\alpha$
a22	No. moles N_2H_4(l) thermally decomposed	$\varepsilon[0.00426(1-\gamma)(\gamma^*)\alpha+0.0008156\gamma^*\alpha\text{-a}21]$
a23	No. moles N_2H_4(l) vaporized	$\eta[0.00426(1-\gamma)(\gamma^*)\alpha+0.0008156\gamma^*\alpha\text{-a}21]$
a24	No. moles LOX reacted	$0.3203\gamma 1\gamma 1^*\alpha$
a25	No. moles LOX vaporized	$0.3203(1-\gamma 1)(\gamma 1^*)\alpha$
	OTHER USEFUL PARAMETER DEFINITIONS	VALUE
	No. moles LOX consumed in flight	$0.3203(1-\gamma 1^*)$
	No. moles RP-1 consumed in flight	$0.3346(1-\gamma 1^*)$
	No. moles NH_4ClO_4 consumed in flight	$0.0965(1-\delta^*)$
	No. moles $CH_{1.622}$ consumed in flight	$0.1341(1-\delta^*)$
	No. moles Al consumed in flight	$0.1156(1-\delta^*)$

TABLE 21. THERMOCHEMICAL MODEL, DELTA II (CONTINUED).

PRODUCT COEFFICIENT	DEFINITION	VALUE
b1	No. moles CO_2 formed by reaction	a1(0.0808)+a24(0.3333)+a12(0.3082)
b2	No. moles CO_2 formed by UDMH-air burn	a17(2.000)
b3	No. moles CO_2 formed by RP-1-air burn	a9(1.000)
b4	No. moles CO formed by reaction	a1(1.2974)+a24(0.6667)+a12(0.3727)
b5	No. moles H_2O formed by reaction	a1(0.7803)+a24(0.6667)+a12(2.6389)
b6	No. moles H_2O formed by N_2H_4-air burn	a21(2.000)
b7	No. moles H_2O formed by UDMH air-burn	a17(4.000)
b8	No. moles H_2O formed by RP-1-air burn	a9(1.000)
b9	No. moles H_2O formed in solids cloud	a1(1.8315)-b11
b10	No. moles H_2 formed by liquids	a24(0.3333)
b11	No. moles H_2 formed by solids IF: 2a5 > a1(1.8315); THEN: b11 = 0	a1(1.8315)-2a5
b12	No. moles H_2 formed by N_2H_4 monodecomposition	a22(0.5000)
b13	No. moles N_2 formed by reaction	a1(0.4978)+a12(1.9402)
b14	No. moles N_2 formed by N_2H_4 monodecomposition	a22(0.5000)
b15	No. moles N_2 formed by N_2H_4-air burn	a21(1.000)
b16	No. moles N_2 formed by UDMH decomposition	a18(1.000)
b17	No. moles N_2 formed by UDMH-air burn	a17(1.000)
b18	No. moles N_2 formed by N_2O_4 decomposition	a14(1.000)
b19	No. moles N_2 entrained in liquid cloud	a6
b20	No. moles N_2 entrained in solid cloud	a7
b21	No. moles HCl formed by reaction	a1(0.9679)(1-0.5σ)
b22	No. moles Al_2O_3 formed by reaction	a1(0.5739)
b23	No. moles NO formed by reaction	a12(0.0745)
b24	No. moles O_2 formed by reaction	a12(0.1456)
b25	No. moles O_2 vaporized	a25
b26	No. moles O_2 entrained in solid cloud	a5-0.5b9
b27	No. moles O_2 entrained in liquid cloud	a4-1.500a9-4a17-a21
b28	No. moles O_2 formed by N_2O_4 thermal decomposition	a14(2.000)
b29	No. moles NH_3 formed by N_2H_4 monodecomposition	a22(1.000)
b30	No. moles N_2H_4 vaporized	a23
b31	No. moles CH_4 formed by UDMH thermal decomposition	a18(2.000)
b32	No. moles UDMH vaporized	a19
b33	No. moles C_2H_4 formed by RP-1 decomposition	a10(0.5000)
b34	No. moles RP-1 vaporized as $C_{12}H_{26}$	0.08333a11
b35	No. moles N_2O_4 vaporized	a15(1-κ)
b36	No. moles NO_2 formed from N_2O_4 vapor	a15(κ)(2.000)
b37	No. moles HNO_3 formed	a13
b38	No. moles NOCl formed	a13

TABLE 21. THERMOCHEMICAL MODEL, DELTA II (CONCLUDED).

SUMMARY	VALUE
REACTANTS	
moles NH_4ClO_4 reacted	a1
moles $CH_{1.622}$ reacted	a2
moles Al reacted	a3
moles O_2(l) reacted or vaporized	a24+a25
moles O_2(g) entrained	a4+a5
moles N_2 entrained	a6+a7
moles RP-1 reacted, combusted, decomposed, or vaporized	a8+a9+a10+a11
moles N_2O_4 reacted, decomposed, or vaporized	a12+a13+a14+a15
moles UDMH reacted, combusted, decomposed, or vaporized	a16+a17+a18+a19
moles hydrazine reacted, combusted,decomposed,or vaporized	a20+a21+a22+a23
PRODUCTS	
moles CO_2 formed	b1+b2+b3
moles CO formed	b4
moles H_2O formed	b5+b6+b7+b8+b9
moles H_2 formed	b10+b11+b12
moles N_2 formed	b13+b14+b15+b16+b17+b18+b19+b20
moles HCl formed	b21
moles Al_2O_3 formed	b22
moles NO formed	b23
moles O_2 formed, vaporized, or entrained	b24+b25+b26+b27+b28
moles NH_3 formed	b29
moles N_2H_4 vaporized	b30
moles CH_4 formed	b31
moles UDMH vaporized	b32
moles C_2H_4 formed	b33
moles RP-1 vaporized as $C_{12}H_{26}$	b34
moles N_2O_4 vaporized	b35
moles NO_2 formed	b36
moles HNO_3 formed	b37
moles NOCl formed	b38

Equations used to determine fireball parameters for an accident involving the Delta II launch vehicle, obtained from data in Table 21 and thermodynamic data reported in Table 7, are identical to those reported in Equations (98) through (103) with the following exceptions:

The scaling factor for the upper (liquids) cloud is calculated as:

$$SF = \frac{146{,}200 \text{ lb LOX} \times 453.59 \text{ g/lb}}{31.999 \text{ g/mole} \times 0.3203 \text{ mole}} = 6.4702\text{x}10^6 \qquad (109)$$

The scaling factor for the lower (solids) cloud is calculated as:

$$SF = \frac{161{,}611 \text{ lb AP} \times 453.59 \text{ g/lb}}{117.489 \text{ g/mole} \times 0.0965 \text{ mole}} = 6.4656\text{x}10^6 \qquad (110)$$

Fireball size for the upper (liquids) cloud is calculated using Equation (102), in which W_b includes the weight in pounds of all liquid and solid propellants, but does not include the weight of entrained air.

Fireball size for the lower (solids) cloud is calculated using Equation (68), in which W_g includes the weight of combustion gases and entrained air, but neglects solid or liquid condensates such as Al_2O_3 and Fe_2O_3.

Total heat release for the upper (liquids) cloud is calculated as:

$$\text{Total Heat Release} = \Delta H_{rxn,\,upper} \times SF \tag{111}$$

where: $\Delta H_{rxn,upper}$ = The heat of reaction calculated using the coefficients specified in Table 21, and incorporating values of the variables consistent with the upper cloud for a Delta II launch vehicle accident. This is the heat of reaction for liquid oxygen reactant corresponding to $\alpha\gamma 1*(0.3203)$ gram moles.

Total heat release for the lower (solids) cloud is calculated as:

$$\text{Total Heat Release} = \Delta H_{rxn,\,lower} \times SF \tag{112}$$

where: $\Delta H_{rxn,lower}$ = The heat of reaction calculated using the coefficients specified in Table 21, and incorporating values of the variables consistent with the lower cloud for a Delta II launch vehicle accident. This is equivalent to the heat of reaction of ammonium perchlorate reactant corresponding to $\beta\delta\delta*(0.0965)$ gram moles.

4. Default Values and Suggested Ranges.

Table 22 shows the suggested values of the 22 input variables for a Delta II on-pad abort (Case 1), for both the upper and lower clouds. Table 23 shows a set of values for a hypothetical in-flight abort incorporating air entrainment (Case 2) for both the upper and lower clouds. Each table contains variable ranges, covering all accident conditions. In the absence of other derived data, the variable values in Case 1 are considered the nominal default values for atmospheric dispersion modeling.

TABLE 22. TEST CASE VALUES, DELTA II MODEL.
TEST CASE 1 ON-PAD ABORT, CONFINED BY GROUND SURFACE, NO AIR ENTRAINMENT IN LIQUID CLOUD.

Variable	Expected Range	Upper Cloud	Lower Cloud
s	0-60	0.00	0.00
A	0-10000	0.00	0.00
α	0.00-1.00	1.00	0.00
β	0.00-1.00	0.10	0.90
δ	0.00-1.00	1.00	1.00
δ*	0.39-1.00	1.00	1.00
γ	0.10-0.40	0.229	0.229
γ*	0.00-1.00	1.00	1.00
γ1	0.10-0.70	0.44	0.44
γ1*	0.78-1.00	1.00	1.00
ζ	0.00-3.00	0.00	0.00
ε	0.00-1.00	0.94	0.94
η	0.00-1.00	0.06	0.06
ξ	0.00-1.00	0.70	0.70
ι	0.00-1.00	0.30	0.30
κ	0.18-1.00	1.00	1.00
λ	0.00-1.00	0.35	0.35
μ	0.00-1.00	0.75	0.75
υ	0.00-1.00	0.25	0.25
π	0.00-1.00	0.00	1.00
ρ	0.00-30.00	2.9248	2.9248
σ	0.00-1.00	1.00	0.00

TABLE 23. TEST CASE VALUES, DELTA II MODEL.
TEST CASE 2, ABORT AT 5000 FEET, COMMAND DESTRUCT,
35 PERCENT AIR ENTRAINMENT LIQUIDS.

Variable	Expected Range	Upper Cloud	Lower Cloud
s	0-60	25	25
A	0-10000	5000	5000
α	0.00-1.00	1.00	0.00
β	0.00-1.00	0.05	0.95
δ	0.00-1.00	1.00	1.00
δ*	0.39-1.00	0.74483	0.74483
γ	0.10-0.40	0.232	0.232
γ*	0.00-1.00	1.00	1.00
γ1	0.10-0.70	0.44	0.44
γ1*	0.78-1.00	0.90816	0.90816
ζ	0.00-3.00	0.28756	0.28756
ε	0.00-1.00	0.70	0.70
η	0.00-1.00	0.30	0.30
ξ	0.00-1.00	0.50	0.50
ι	0.00-1.00	0.50	0.50
κ	0.18-1.00	1.00	1.00
λ	0.00-1.00	0.10	0.10
μ	0.00-1.00	0.50	0.50
υ	0.00-1.00	0.50	0.50
π	0.00-1.00	0.00	1.00
ρ	0.00-30.00	10.928	10.928
σ	0.00-1.00	1.00	0.00

5. Results

Fireball data for the two test cases identified in Tables 22 and 23 are presented in Tables 24 and 25, respectively. These data include chemical composition, fireball size, total heat released, and adiabatic flame temperature. Computer spreadsheets showing the calculations for these two test cases are contained in Appendix F.

TABLE 24. SOURCE STRENGTH SUMMARY - DELTA II LAUNCH VEHICLE-CASE 1.

Abort Condition: On-Pad Accident; Confined by Ground Surface (CBGS); 0 Air Entrainment (Upper Cloud)

Propellant Loading:	Liquid Oxygen	146,200 lbs
	RP-1	66,700 lbs
	Nitrogen Tetroxide	8,759 lbs
	Aerozine-50	4,640 lbs
	Ammonium Perchlorate	161,611 lbs
	HTPB	26,099 lbs
	Aluminum	44,490 lbs

	UPPER CLOUD		**LOWER CLOUD**	
Constituent	Mole %	Mass, lbs	Mole %	Mass, lbs
Reactants				
$NH_4ClO_4(s)$	1.37	16,173	15.36	145,450
$CH_{1.622}(s)$	1.90	2,610	21.34	23,476
Al(s)	1.64	4,449	18.39	40,015
$O_2(l)$	45.49	146,200	0.00	0
$CH_{1.95}(l)$	47.53	66,706	0.00	0
$N_2O_4(l)$	0.95	8,794	0.00	0
$C_2H_8N_2(l)$	0.38	2,320	0.00	0
$N_2H_4(l)$	0.72	2,320	0.00	0
$O_2(g)$	0.00	0	9.43	24,332
$N_2(g)$	0.00	0	35.48	80,132
TOTAL	99.99	249,572	100.00	313,405
Products				
$CO_2(g)$	7.73	30,275	0.97	4,402
CO(g)	17.17	42,772	15.56	44,989
$H_2O(g)$	16.93	27,121	24.08	44,799
$H_2(g)$	10.68	1,914	7.23	1,505
$N_2(g)$	1.82	4,538	33.67	97,395
HCl(g)	0.75	2,429	11.61	43,689
Al_2O_3	0.89	8,055	6.88	72,441
NO(g)	0.02	49	0.00	0
$O_2(g)$	28.84	82,083	0.00	0
$NH_3(g)$	0.62	936	0.00	0
$CH_4(g)$	0.49	700	0.00	0
$C_2H_4(g)$	11.65	29,063	0.00	0
$NO_2(g)$	0.07	291	0.00	0
$HNO_3(g)$	0.77	4,337	0.00	0
NOCl(g)	0.77	4,505	0.00	0
Vaporized Propellants				
$C_2H_8N_2(g)$	0.11	562	0.00	0
$N_2H_4(g)$	0.04	112	0.00	0
$N_2O_4(g)$	0.00	0	0.00	0
RP-1(g) as $C_{12}H_{26}$	0.65	9,803	0.00	0
TOTAL	100.00	249,545	100.00	309,220

TABLE 24. SOURCE STRENGTH SUMMARY - DELTA II LAUNCH VEHICLE CASE 1 (CONCLUDED).

Abort Condition: On-Pad Accident; Confined by Ground Surface (CBGS); 0 air entrainment (upper cloud)		
	UPPER CLOUD	**LOWER CLOUD**
Adiabatic Flame Temperature (K)	1882	3807
Average Molecular Weight (g/mole)	28.06	29.95 24.63 (gases only)
Fireball Size		
Diameter (feet)	522	451
Volume (cubic feet)	7.45E+07	4.81E+07
Total Heat Released (calories)	-7.49E+10	-1.80E+11

TABLE 25. SOURCE STRENGTH SUMMARY - DELTA II LAUNCH VEHICLE-CASE 2.

Abort Condition: Abort at 5000 Feet, Command Destruct, 0.35 Pound Air/Pound Liquid Propellants (Upper Cloud)

Propellant Loading:	
Liquid Oxygen	146,200 lbs
RP-1	66,700 lbs
Nitrogen Tetroxide	8,759 lbs
Aerozine-50	4,640 lbs
Ammonium Perchlorate	161,611 lbs
HTPB	26,099 lbs
Aluminum	44,490 lbs

Constituent	UPPER CLOUD Mole %	UPPER CLOUD Mass, lbs	LOWER CLOUD Mole %	LOWER CLOUD Mass, lbs
Reactants				
$NH_4ClO_4(s)$	0.45	6,023	6.89	114,354
$CH_{1.622}(s)$	0.63	972	9.57	18,457
$Al(s)$	0.54	1,657	8.25	31,460
$O_2(l)$	36.48	132,773	0.00	0
$CH_{1.95}(l)$	38.11	60,579	0.00	0
$N_2O_4(l)$	0.84	8,794	0.00	0
$C_2H_8N_2(l)$	0.34	2,320	0.00	0
$N_2H_4(l)$	0.64	2,320	0.00	0
$O_2(g)$	4.61	16,793	15.81	71,475
$N_2(g)$	17.36	55,305	59.48	235,388
TOTAL	100.00	287,536	100.00	471,134
Products				
$CO_2(g)$	7.95	34,844	0.50	3,461
$CO(g)$	12.97	36,188	8.09	35,370
$H_2O(g)$	15.02	26,950	16.28	45,796
$H_2(g)$	7.25	1,455	0.00	0
$N_2(g)$	20.94	58,433	56.92	248,961
$HCl(g)$	0.25	905	6.03	34,349
Al_2O_3	0.30	3,000	3.58	56,954
$NO(g)$	0.02	50	0.00	0
$O_2(g)$	26.09	83,159	8.60	42,954
$NH_3(g)$	0.39	664	0.00	0
$CH_4(g)$	0.30	477	0.00	0
$C_2H_4(g)$	5.87	16,407	0.00	0
$NO_2(g)$	0.86	3,956	0.00	0
$HNO_3(g)$	0.26	1,615	0.00	0
$NOCl(g)$	0.26	1,678	0.00	0
Vaporized Propellants				
$C_2H_8N_2(g)$	0.15	893	0.00	0
$N_2H_4(g)$	0.17	535	0.00	0
$N_2O_4(g)$	0.00	0	0.00	0
RP-1(g) as $C_{12}H_{26}$	0.98	16,603	0.00	0
TOTAL	100.03	287,812	100.00	467,845

TABLE 25. SOURCE STRENGTH SUMMARY-DELTA II LAUNCH VEHICLE, CASE 2 (CONCLUDED).

Abort Condition: Abort at 5000 Feet, Command Destruct, 0.35 Pound Air/Pound Liquid Propellants (Upper Cloud).		
	UPPER CLOUD	**LOWER CLOUD**
Adiabatic Flame Temperature (K)	1790	2625
Average Molecular Weight (g/mole)	28.89	29.96 27.29 (gases only)
Fireball Size		
Diameter (feet)	497	463
Volume (cubic feet)	6.45E+07	5.19E+07
Total Heat Released (calories)	-7.44E+10	-1.57E+11

G. SOURCE MODEL, TITAN IV

1. Propellant Loading

The nominal propellant loading and consumption rates for the liquid rocket propellants (Aerozine-50 and nitrogen tetroxide) and the Solid Rocket Motor (SRM) propellant on the Titan IV launch vehicle are shown in Table 26. Data for this table are taken from the Martin Marietta Corporation[10,11].

TABLE 26. TITAN IV PROPELLANT LOADING AND CONSUMPTION RATES.

Stage	Parameter	Value	Units
1st Stage*	Loaded Weight, Nitrogen Tetroxide	226,617	pounds
	Loaded Weight, Aerozine-50	119,134	pounds
2nd Stage*	Loaded Weight, Nitrogen Tetroxide	49,164	pounds
	Loaded Weight, Aerozine-50	27,891	pounds
Thrust Vector Control (TVC)**	Loaded Weight, Nitrogen Tetroxide	2 tanks @ 8,424 pounds/tank	pounds
Solids	Loaded Weight,UTP-3001B	2 motors @ 591,000 pounds/motor	pounds
Solids	Burn Rate	2 motors @ 5,382 pounds/second-motor	pounds/second (each motor)

Notes: * Stage I,II liquid propellant loadings are based on West Coast (Vandenburg AFB) launch inclinations. Loadings for launches conducted at East Coast (Kennedy Space Center) are slightly different. Burn rates for liquid rocket propellants are not supplied, because initiation of these engines do not occur below 10,000 feet altitude.

** Nominal loading. An optional loading is two tanks at 10,024 pounds N_2O_4 per tank. Four or five launches are planned using this optional configuration.

Molar coefficients of reactants (hydrazine, unsymmetrical dimethylhydrazine, nitrogen tetroxide, ammonium perchlorate, aluminum, and PBAN) are included in Table 27.

[10]Williams, Henry. Martin Marietta Titan IV Program Office. Private Communication.
[11]Langhenry, Mark. Martin Marietta Propulsion Department. Private Communication.

TABLE 27. MOLAR COEFFICIENTS USED FOR TITAN IV MODELING

Reactant	Formula	Weight, lbs.	Molecular Weight (g/g-mole)	actual g-moles	normalized g-moles
Ammonium Perchlorate	NH_4ClO_4	797,968	117.489	3,080,716	0.2055
PBAN	$CH_{1.427}O_{.095}N_{.021}$	190,538	15.263	5,662,460	0.3777
Aluminum	Al	190,538	26.982	3,203,103	0.2137
Iron Oxide	Fe_2O_3	2,955	159.692	8,393	0.000559
Nitrogen Tetroxide (main engine)	N_2O_4	275,781	92.016	1,359,454	0.0907
Nitrogen Tetroxide (TVC)*	N_2O_4	16,848	92.016	83,052	0.0055
Hydrazine	N_2H_4	73,512	32.045	1,040,546	0.0694
UDMH	$C_2H_8N_2$	73,512	60.102	554,795	0.0370

Notes:
1. Nitrogen tetroxide from thrust vector control tank, and non-stoichiometric amounts of hydrazine and UDMH are not combusted in the normal bipropellant reaction, but are treated as excess propellants which may react with air, thermally decompose, or vaporize.
2. Normalized g-moles (mole fraction of reactants) are determined by dividing actual g-moles by the total amount of all propellants, including propellants in TVC and Aerozine-50 reacting non-stoichiometrically. This latter value is 1.4992×10^7, and is also the scaling factor.
3. Hydrazine amount includes 61,306 pounds hydrazine reacting stoichiometrically (0.0579 normalized g-moles) plus 12,206 pounds hydrazine (0.0115 normalized g-moles) excess for fuel-rich propellant loading.
4. UDMH amount includes 61,304 pounds UDMH reacting stoichiometrically (0.0309 normalized g-moles) plus 12,208 pounds UDMH (0.0061 normalized g-moles) excess for fuel-rich propellant loading.

2. Propellant Combustion Reactions.

Propellant combustion reactions used to prepare the Titan IV Source Model are listed in the following equations. The equations are simplified reactions in which free radicals combine to form more stable chemical compounds, and residual hydrogen and oxygen react to form water vapor.

a. Aerozine-50 and Nitrogen Tetroxide

$$0.6522\ N_2H_4 + 0.3478\ C_2H_8N_2 + 1.0217\ N_2O_4 \rightarrow 2.6962\ H_2O + 1.9823\ N_2 + 0.3149\ CO_2 + 0.3808\ CO + 0.0761\ NO + 0.1488\ O_2 \quad (113)$$

$T_F = 3763$ K

$\Delta H_{rxn} = -2.01 \times 10^5$ calories

b. SRM Solid Propellant

$$1.0000\ NH_4ClO_4 + 1.8374\ CH_{1.427}O_{.095}N_{.021} + 1.0397\ Al + 0.0028\ Fe_2O_3 \rightarrow 0.0875\ CO_2 + 1.7511\ CO + 0.6955\ H_2O + 2.1168\ H_2 + 0.5178\ N_2 + 0.9937\ HCl + 0.5132\ Al_2O_3(l) + 0.0028\ Fe_2O_3(s) \qquad (114)$$

$T_F = 3559$ K

$\Delta H_{rxn} = -2.35 \times 10^5$ calories

Notes: 1. $CH_{1.427}O_{.095}N_{.021}$ is a calculated empirical formula for the combination of the PBAN polymer, Nadic Methyl Anhydride (NMA) liquid epoxy curative, and Dioctyl Adipate (DOA) plasticizer. Its calculated heat of formation is -3434 calories/g-mole. The species is called PBAN(composite) in all future thermochemical references.

2. The stoichiometry for the Titan IV PBAN propellant is slightly different than that previously used for the Titan 34D PBAN propellant reported in Reference 6. The formulation used by the manufacturer (United Technologies Chemical Systems Division) is slightly different for the Titan IV motors.

3. Mathematical Formulation of the Titan IV Chemical Source Model.

The equations used to determine reactant and product compositions involving the Titan IV launch vehicle system are presented in Table 28. The equations are comprised of the 18 variables developed for the Titan IV model, the values of which are determined by the specific accident conditions and assumptions used. The stoichiometry of the reactants is taken from the normalized molar loading presented in Table 27. Reactants and products are modified by one or more of the eighteen variables to determine their contributions to the explosive event. Establishment of a mass balance within the accuracy of the source model is verified. In the case of the Titan IV vehicle, two combustion clouds are generated by the model: an upper cloud consisting of products in the liquid propellant reactions; and a lower cloud consisting of the combustion products of the solid propellants and containing entrained air.

TABLE 28. THERMOCHEMICAL MODEL, TITAN IV.

VARIABLE	DEFINITION	UNITS
s	Time of Abort (from launch)	seconds
A	Altitude at Abort	feet
α	Fraction Total Liquids in Cloud	moles liquid propellant in cloud/total moles of liquid propellant in all clouds
β	Fraction Total Solids in Cloud	moles solid propellant in cloud/total moles of solid propellant in all clouds
δ	Solid Propellant Reactivity Ratio	moles solid propellant reacted/total moles at abort
δ^*	Solid Propellant Consumption Ratio	moles solid propellant at abort/total moles loaded
γ	Liquid Propellant Reactivity Ratio, N_2O_4/A-50	moles N_2O_4 & A-50 reacted/total moles at abort
γ^*	Liquid Propellant Consumption Ratio, N_2O_4/A-50	moles N_2O_4 & A-50 at abort/total moles loaded
ζ	Air Entrainment Ratio, Liquids	moles air entrained/total moles liquids at abort
ε	Fraction Excess Hydrazine Monodecomposed (after air burning)	moles hydrazine decomposed/total moles hydrazine available
η	Fraction Excess Hydrazine Vaporized or Condensed	moles hydrazine vaporized/total moles hydrazine available
ξ	Fraction Excess UDMH Thermally Decomposed (after air burning)	moles UDMH decomposed/total moles UDMH available
ι	Fraction Excess UDMH Vaporized or Condensed	moles UDMH vaporized/total moles UDMH available
κ	Fraction Excess Nitrogen Tetroxide Converted to NO_2	moles N_2O_4 converted to 2 moles NO_2/total moles N_2O_4 available
λ	Fraction Excess NO_2 Thermally Decomposed	moles NO_2 converted to 0.5 moles N_2 and 1.0 mole O_2/total moles NO_2 available
π	Fraction of Solids which Entrain Air	moles of solids entraining air/total moles solids available
ρ	Air Entrainment Ratio, Solids	moles of air entrained/moles ammonium perchlorate available
σ	HCl reactivity	"dummy variable": $\alpha=0,\sigma=0$; $\alpha>0,\sigma=1$

TABLE 28. THERMOCHEMICAL MODEL, TITAN IV (CONTINUED).

REACTANT COEFFICIENT	DEFINITION	VALUE
a1	No. moles NH_4ClO_4(s) reacted	$0.2055\beta\delta\delta^*$
a2	No. moles $CH_{1.427}O_{.095}N_{.021}$(s) reacted	$0.3777\beta\delta\delta^*$
a3	No. moles Al(s) reacted	$0.2137\beta\delta\delta^*$
a4	No. moles Fe_2O_3(s) reacted	$0.000559\beta\delta\delta^*$
a5	No. moles O_2 entrained in liquid	$0.0425\zeta\gamma^*\alpha$
a6	No. moles O_2 entrained in solid	$0.21(a1)\rho\pi$
a7	No. moles N_2 entrained in liquid	$0.1601\zeta\gamma^*\alpha$
a8	No. moles N_2 entrained in solid	$0.79(a1)\rho\pi$
a9	No. moles N_2O_4(l) reacted	$0.0907\gamma\gamma^*\alpha$
a10	No. moles N_2O_4(g) reacted with HCl	$\sigma(0.5000)(a1)$
a11	No. moles N_2O_4(g) decomposed to N_2 + 2 O_2	$\lambda[0.0907(1-\gamma)\gamma^*\alpha+0.0055\gamma^*\alpha-\sigma(0.5000)a1]$
a12	No. moles N_2O_4 vaporized to $2NO_2$	$(1-\lambda)[0.0907(1-\gamma)\gamma^*\alpha+0.0055\gamma^*\alpha-\sigma(0.5000)a1]$
a13	No. moles UDMH(l) reacted	$0.0309\gamma\gamma^*\alpha$
a14	No. moles UDMH(l) combusted in air IF: $a14 > 0.0309(1-\gamma)(\gamma^*)+0.0061\gamma^*$; THEN: $a14 = 0.0309(1-\gamma)(\gamma^*)+0.0061\gamma^*$	$0.00425\zeta\gamma^*\alpha$
a15	No. moles UDMH (l) thermally decomposed	$\xi[0.0309(1-\gamma)(\gamma^*)\alpha+0.0061\gamma^*\alpha\text{-}a14]$
a16	No. moles UDMH (l) vaporized	$\iota[0.0309(1-\gamma)(\gamma^*)\alpha+0.0061\gamma^*\alpha\text{-}a14]$
a17	No. moles N_2H_4(l) reacted	$0.0579\gamma\gamma^*\alpha$
a18	No. moles N_2H_4(l) combusted in air IF: $a18>0.0579(1-\gamma)(\gamma^*)+0.0115\gamma^*$; THEN: $a18 = 0.0579(1-\gamma)(\gamma^*)+0.0115\gamma^*$	$0.00425\zeta\gamma^*\alpha$
a19	No. moles N_2H_4(l) thermally decomposed	$\varepsilon[0.0579(1-\gamma)(\gamma^*)\alpha+0.0115\gamma^*\alpha\text{-}a18]$
a20	No. moles N_2H_4(l) vaporized	$\eta[0.0579(1-\gamma)(\gamma^*)\alpha+0.0115\gamma^*\alpha\text{-}a18]$
	OTHER USEFUL PARAMETER DEFINITIONS	VALUE
	No. moles NH_4ClO_4 consumed in flight	$0.2055(1-\delta^*)$
	No. moles $CH_{1.427}O_{.095}N_{.021}$ consumed in flight	$0.3777(1-\delta^*)$
	No. moles Al consumed in flight	$0.2137(1-\delta^*)$

TABLE 28. THERMOCHEMICAL MODEL, TITAN IV (CONTINUED).

PRODUCT COEFFICIENT	DEFINITION	VALUE
b1	No. moles CO_2 formed by reaction	a1(0.0875)+a9(0.3082)
b2	No. moles CO_2 formed by UDMH-air burn	a14(2.000)
b3	No. moles CO formed by reaction	a1(1.7511)+a9(0.3727)
b4	No. moles H_2O formed by reaction	a1(0.6955)+a9(2.6389)
b5	No. moles H_2O formed by N_2H_4-air burn	a18(2.000)
b6	No. moles H_2O formed by UDMH air-burn	a14(4.000)
b7	No. moles H_2O formed in solids cloud	a1(2.1168)-b8
b8	No. moles H_2 formed by solids IF: 2a6 > a1(2.1168); THEN: b8 = 0	a1(2.1168)-2a6
b9	No. moles H_2 formed by N_2H_4 monodecomposition	a19(0.5000)
b10	No. moles N_2 formed by reaction	a1(0.5178)+a9(1.9402)
b11	No. moles N_2 formed by N_2H_4 monodecomposition	a19(0.5000)
b12	No. moles N_2 formed by N_2H_4-air burn	a18(1.000)
b13	No. moles N_2 formed by UDMH decomposition	a15(1.000)
b14	No. moles N_2 formed by UDMH-air burn	a14(1.000)
b15	No. moles N_2 formed by N_2O_4 decomposition	a11(1.000)
b16	No. moles N_2 entrained in liquid cloud	a7
b17	No. moles N_2 entrained in solid cloud	a8
b18	No. moles HCl formed by reaction	a1(0.9937)(1-0.5σ)
b19	No. moles Al_2O_3 formed by reaction	a1(0.5132)
b20	No. moles NO formed by reaction	a9(0.0745)
b21	No. moles O_2 formed by reaction	a9(0.1456)
b22	No. moles O_2 entrained in solid cloud	a6-0.5b7
b23	No. moles O_2 entrained in liquid cloud	a5-4a14-a18
b24	No. moles O_2 formed by N_2O_4 thermal decomposition	a11(2.000)
b25	No. moles NH_3 formed by N_2H_4 monodecomposition	a19(1.000)
b26	No. moles N_2H_4 vaporized	a20
b27	No. moles CH_4 formed by UDMH thermal decomposition	a15(2.000)
b28	No. moles UDMH vaporized	a16
b29	No. moles N_2O_4 vaporized	a12(1-κ)
b30	No. moles NO_2 formed from N_2O_4 vapor	a12(κ)(2.000)
b31	No. moles HNO_3 formed	a10
b32	No. moles NOCl formed	a10
b33	No. moles Fe_2O_3 formed	a4

TABLE 28. THERMOCHEMICAL MODEL, TITAN IV (CONCLUDED).

SUMMARY	VALUE
REACTANTS	
moles NH_4ClO_4 reacted	a1
moles $CH_{1.427}O_{.095}N_{.021}$ reacted	a2
moles Al reacted	a3
moles Fe_2O_3 reacted	a4
moles O_2 entrained	a5+a6
moles N_2 entrained	a7+a8
moles N_2O_4 reacted, decomposed, or vaporized	a9+a10+a11+a12
moles UDMH reacted, combusted, decomposed, or vaporized	a13+a14+a15+a16
moles hydrazine reacted, combusted,decomposed,or vaporized	a17+a18+a19+a20
PRODUCTS	
moles CO_2 formed	b1+b2
moles CO formed	b3
moles H_2O formed	b4+b5+b6+b7
moles H_2 formed	b8+b9
moles N_2 formed	b10+b11+b12+b13+b14+b15+b16+b17
moles HCl formed	b18
moles Al_2O_3 formed	b19
moles NO formed	b20
moles O_2 formed or entrained	b21+b22+b23+b24
moles NH_3 formed	b25
moles N_2H_4 vaporized	b26
moles CH_4 formed	b27
moles UDMH vaporized	b28
moles N_2O_4 vaporized	b29
moles NO_2 formed	b30
moles HNO_3 formed	b31
moles NOCl formed	b32
moles Fe_2O_3 formed	b33

Equations used to determine fireball parameters involving the Titan IV launch vehicle, taken from data in Table 28 and thermodynamic data reported in Table 12, are identical to those reported in Equations (93) through (103) with the following exceptions:

The scaling factor for the upper (liquids) cloud is calculated as:

$$SF = \frac{275{,}781\ \text{lb N2O4} \times 453.59\ \text{g/lb}}{92.016\ \text{g/mole} \times 0.0907\ \text{mole}} = 1.4988\text{x}10^7 \tag{115}$$

The scaling factor for the lower (solids) cloud is calculated as:

$$SF = \frac{797{,}968\ \text{lb AP} \times 453.59\ \text{g/lb}}{117.489\ \text{g/mole} \times 0.2055\ \text{mole}} = 1.4991\text{x}10^7 \tag{116}$$

Fireball size for the upper (liquids) cloud is calculated using Equation (102), in which W_b includes the weight in pounds of all liquid and solid propellants, but does not include the weight of entrained air.

Fireball size for the lower (solids) cloud is calculated using Equation (68), in which W_g includes the weight of combustion gases and entrained air, but neglects solid or liquid condensates such as Al_2O_3 and Fe_2O_3.

Total heat release for the upper (liquids) cloud is calculated as:

$$\text{Total Heat Release} = \Delta H_{rxn,\,upper} \times SF \qquad (117)$$

Where $\Delta H_{rxn,upper}$ = The heat of reaction calculated using the coefficients specified in Table 28, and incorporating values of the variables consistent with the upper cloud from a Titan IV launch vehicle accident. This is the heat of reaction for nitrogen tetroxide reactant corresponding to $\alpha\gamma$*(0.0907+0.0055) gram moles.

Total Heat Release for the lower (solids) cloud is calculated as:

$$\text{Total Heat Release} = \Delta H_{rxn,\,lower} \times SF \qquad (118)$$

Where $\Delta H_{rxn,lower}$ = The heat of reaction calculated using the coefficients specified in Table 28, and incorporating the values of the variables consistent with the lower cloud from a Titan IV launch vehicle accident. This is the heat of reaction for ammonium perchlorate reactant corresponding to $\beta\delta\delta$*(0.2055) gram moles.

4. Default Values and Suggested Ranges.

Table 29 shows the suggested values of the 18 input variables for a Titan IV on-pad abort (Case 1), for both the upper and lower clouds. Table 30 shows a set of values for a hypothetical in-flight abort incorporating air entrainment (Case 2) for both the upper and lower clouds. Each table contains variable ranges covering all accident conditions. In the absence of other derived data, the variable values in Case 1 are considered the nominal default values for atmospheric dispersion modeling.

TABLE 29. TEST CASE VALUES, TITAN IV MODEL.
TEST CASE 1 ON-PAD ABORT, CONFINED BY GROUND SURFACE, NO AIR ENTRAINMENT IN LIQUID CLOUD.

Variable	Expected Range	Upper Cloud	Lower Cloud
s	0-60	0.00	0.00
A	0-10000	0.00	0.00
α	0.00-1.00	1.00	0.00
β	0.00-1.00	0.10	0.90
δ	0.00-1.00	1.00	1.00
δ*	0.39-1.00	1.00	1.00
γ	0.10-0.40	0.229	0.229
γ*	0.00-1.00	1.00	1.00
ζ	0.00-3.00	0.00	0.00
ε	0.00-1.00	0.94	0.94
η	0.00-1.00	0.06	0.06
ξ	0.00-1.00	0.70	0.70
ι	0.00-1.00	0.30	0.30
κ	0.18-1.00	1.00	1.00
λ	0.00-1.00	0.35	0.35
π	0.00-1.00	0.00	1.00
ρ	0.00-30.00	3.0162	3.0162
σ	0.00-1.00	1.00	0.00

TABLE 30. TEST CASE VALUES, TITAN IV MODEL.
TEST CASE 2 ABORT AT 5000 FEET, COMMAND DESTRUCT,
35 PERCENT AIR ENTRAINMENT LIQUIDS.

Variable	Expected Range	Upper Cloud	Lower Cloud
s	0-60	25	25
A	0-10000	5000	5000
α	0.00-1.00	1.00	0.00
β	0.00-1.00	0.05	0.95
δ	0.00-1.00	1.00	1.00
δ*	0.39-1.00	0.7723	0.7723
γ	0.10-0.40	0.232	0.232
γ*	0.00-1.00	1.00	1.00
ζ	0.00-3.00	0.35	0.35
ε	0.00-1.00	0.70	0.70
η	0.00-1.00	0.30	0.30
ξ	0.00-1.00	0.50	0.50
ι	0.00-1.00	0.50	0.50
κ	0.18-1.00	1.00	1.00
λ	0.00-1.00	0.10	0.10
π	0.00-1.00	0.00	1.00
ρ	0.00-30.00	5.0959	5.0959
σ	0.00-1.00	1.00	0.00

5. Results

Fireball data for the two test cases identified in Tables 29 and 30 are presented in Tables 31 and 32, respectively. These data include chemical composition, fireball size, total heat released, and adiabatic flame temperature. Computer spreadsheets showing the calculations for these two test cases are contained in Appendix F.

TABLE 31. SOURCE STRENGTH SUMMARY - TITAN IV LAUNCH VEHICLE-CASE 1.

Abort Condition: On-Pad Accident; Confined by Ground Surface (CBGS); 0 Air Entrainment (Upper Cloud)

Propellant Loading:		
	Nitrogen Tetroxide (engine)	275,781 lbs
	Nitrogen Tetroxide (TVC)	16,848 lbs
	Aerozine-50	147,025 lbs
	Ammonium Perchlorate	797,968 lbs
	PBAN	190,538 lbs
	Aluminum	190,538 lbs
	Iron Oxide	2,955 lbs

Constituent	UPPER CLOUD Mole %	Mass, lbs	LOWER CLOUD Mole %	Mass, lbs
Reactants				
$NH_4ClO_4(s)$	7.28	79,782	14.53	718,156
$CH_{1.427}O_{.095}N_{.021}(s)$	13.38	19,049	26.70	171,473
$Al(s)$	7.57	19,053	15.10	171,510
$Fe_2O_3(s)$	0.02	295	0.04	2,655
$N_2O_4(l)$	34.07	292,504	0.00	0
$C_2H_8N_2(l)$	13.10	73,483	0.00	0
$N_2H_4(l)$	24.58	73,487	0.00	0
$O_2(g)$	0.00	0	9.20	123,888
$N_2(g)$	0.00	0	34.61	408,001
TOTAL	100.00	557,653	100.17	1,595,653
Products				
$CO_2(g)$	1.38	11,924	0.97	23,539
$CO(g)$	7.35	40,471	19.35	299,810
$H_2O(g)$	11.61	41,136	21.68	216,082
$H_2(g)$	11.74	4,656	9.39	10,475
$N_2(g)$	20.34	112,076	32.04	496,664
$HCl(g)$	1.72	12,302	10.98	221,465
Al_2O_3	1.77	35,533	5.67	319,847
$NO(g)$	0.26	1,534	0.00	0
$O_2(g)$	8.17	51,423	0.00	0
$NH_3(g)$	8.87	29,697	0.00	0
$CH_4(g)$	7.04	22,205	0.00	0
$NO_2(g)$	14.23	128,765	0.00	0
$HNO_3(g)$	1.73	21,395	0.00	0
$NOCl(g)$	1.73	22,225	0.00	0
$Fe_2O_3(s)$	0.01	295	0.03	2,655
Vaporized Propellants				
$C_2H_8N_2(g)$	1.51	17,829	0.00	0
$N_2H_4(g)$	0.57	3,567	0.00	0
$N_2O_4(g)$	0.00	0	0.00	0
TOTAL	100.03	557,033	100.11	1,590,536

TABLE 31. SOURCE STRENGTH SUMMARY - TITAN IV LAUNCH VEHICLE-CASE 1 (CONCLUDED).

Abort Condition: On-Pad Accident; Confined by Ground Surface (CBGS); 0 Air Entrainment (Upper Cloud)		
	UPPER CLOUD	**LOWER CLOUD**
Adiabatic Flame Temperature (K)	1830	3534
Average Molecular Weight (g/mole)	28.32	28.72 24.28 (gases only)
Fireball Size		
Diameter (feet)	673	774
Volume (cubic feet)	1.59E+08	2.42E+08
Total Heat Released (calories)	-1.53E+11	-8.55E+11

TABLE 32. SOURCE STRENGTH SUMMARY - TITAN IV LAUNCH VEHICLE-CASE 2.

Abort Condition: Abort at 5000 Feet, Command Destruct, 0.35 Moles Air/Mole Liquid Propellants (Upper Cloud)

Propellant Loading:	Nitrogen Tetroxide (engine)	275,781 lbs
	Nitrogen Tetroxide (TVC)	16,848 lbs
	Aerozine-50	147,025 lbs
	Ammonium Perchlorate	797,968 lbs
	PBAN	190,538 lbs
	Aluminum	190,538 lbs
	Iron Oxide	2,955 lbs

	UPPER CLOUD		**LOWER CLOUD**	
Constituent	Mole %	Mass, lbs	Mole %	Mass, lbs
Reactants				
$NH_4ClO_4(s)$	2.61	30,809	11.14	585,471
$CH_{1.427}O_{.095}N_{.021}(s)$	4.79	7,356	20.48	139,792
$Al(s)$	2.71	7,358	11.58	139,822
$Fe_2O_3(s)$	0.01	114	0.03	2,165
$N_2O_4(l)$	31.61	292,504	0.00	0
$C_2H_8N_2(l)$	12.16	73,483	0.00	0
$N_2H_4(l)$	22.81	73,487	0.00	0
$O_2(g)$	4.89	15,728	11.92	170,642
$N_2(g)$	18.41	51,870	44.85	561,973
TOTAL	100.00	552,709	100.00	1,599,865
Products				
$CO_2(g)$	1.85	14,768	0.82	19,190
$CO(g)$	3.96	20,121	16.34	244,418
$H_2O(g)$	12.74	41,654	26.24	252,467
$H_2(g)$	6.53	2,389	0.00	0
$N_2(g)$	26.26	133,577	42.40	634,255
$HCl(g)$	0.72	4,750	9.27	180,548
Al_2O_3	0.74	13,722	4.79	260,753
$NO(g)$	0.28	1,554	0.00	0
$O_2(g)$	4.50	26,159	0.11	1,872
$NH_3(g)$	6.94	21,461	0.00	0
$CH_4(g)$	5.16	15,023	0.00	0
$NO_2(g)$	23.32	194,804	0.00	0
$HNO_3(g)$	0.72	8,262	0.00	0
$NOCl(g)$	0.72	8,583	0.00	0
$Fe_2O_3(s)$	0.00	114	0.02	2,165
Vaporized Propellants				
$C_2H_8N_2(g)$	2.58	28,146	0.00	0
$N_2H_4(g)$	2.97	17,307	0.00	0
$N_2O_4(g)$	0.00	0	0.00	0
TOTAL	99.99	552,394	99.99	1,595,668

TABLE 32. SOURCE STRENGTH SUMMARY - TITAN IV LAUNCH VEHICLE-CASE 2 (CONCLUDED).

Abort Condition: Abort at 5000 Feet, Command Destruct, 0.35 Moles Air/Mole Liquid Propellants (Upper Cloud)		
	UPPER CLOUD	**LOWER CLOUD**
Adiabatic Flame Temperature (K)	1407	3494
Average Molecular Weight (g/mole)	30.42	29.88 26.22 (gases only)
Fireball Size		
Diameter (feet)	642	764
Volume (cubic feet)	1.38E+08	2.33E+08
Total Heat Released (calories)	-1.02E+11	-8.08E+11

H. SOURCE MODEL, SOLID PROPELLANTS

1. Propellant Loading

a. Delta II GEMs

Each solid rocket motor contains 25,800 pounds of propellant, and is cast as a single segment. The smallest accident that can occur with the Delta solids involves one motor. Larger scale accidents must contain some multiple of 25,800 pounds of solid propellant.

b. Titan IV SRM

Each solid rocket motor consists of nine segments with a total propellant weight of 591,000 pounds. Each segment contains 65,667 pounds of propellant. The smallest accident that can occur with theTitan IV SRM motors involves one segment. Larger scale accidents must contain some multiple of 65,667 pounds of solid propellant.

2. Propellant Combustion Reactions

The propellant combustion reactions used for modeling solid propellant accidents are identical to those specified in Sections IV F and IV G.

3. Description of Assumptions and Conditions.

a. This model addresses the possibility of an accidental ignition of a solid rocket motor segment or segments during ground handling. Explosion and fragmentation of a fully assembled propulsive motor are not considered in this model.

b. The burn rate of solid propellants at atmospheric pressure is derived from high pressure burn rate equations. This analysis assumes that the burn rate equations are valid at one atmosphere pressure. No other data are available for low pressure burn rates of these propellants.

c. This model assumes the propellant segments are non-propulsive and non-pressurized. The segments burn normally as a single, nonfragmented piece. The grains are tailored to burn neutrally, and inadvertent ignition occurs within the center of the grain as in a normal ignition.

d. Air is expected to be entrained into the solid combustion cloud at 50 percent by mass of the burned propellant. At this time the propellants are completely consumed, the combustion process ceases, and the fireball reaches burnout. The propellant combustion products continue to entrain air and cool as they rise through the atmosphere, but the modeling of this event is beyond the scope of this effort.

4. Variable Definitions, Units, Mathematical Formulation, and Reactant/Product Identification

a. Titan IV Solids Only Model (SRM)

User definable constants:

brsa: Burn Rate of Solid propellant at 1 atmosphere pressure, meters per second
Default: brsa=0.002794

nsia: Number of Segments Involved in the Accident
Default: nsia=1

mss: Mass of Solid propellant per Segment, grams
Default: mss=29,785,743

awt: Average Web Thickness of the grain, meters
Default: awt=1.2

Calculations:

msia: Mass of Solids Involved in the Accident, grams
msia= nsia * mss

gsia: Gram moles of Solid propellant Involved in the Accident
gsia= msia/44.84689

Burn Time: Burn Time= awt/brsa, seconds

Reactants:	Description:
R08S= 0.2577*gsia	Ammonium Perchlorate
R07S= 0.2679*gsia	Aluminum
R10S= 0.4737*gsia	PBAN
R06S= 0.0007*gsia	Iron Oxide
R11E= (msia/28.84)*0.79*0.5	Nitrogen Entrained
R12E= (msia/28.84)*0.21*0.5	Oxygen Entrained

Products:

P30S= 0.0875*R08S	Carbon Dioxide
P31S= 1.7511*R08S	Carbon Monoxide
P33S= 0.6955*R08S	Water
P38S= 0.5178*R08S	Nitrogen
P38E= R11E	Nitrogen Entrained
P43S= 0.9937*R08S	Hydrogen Chloride
P46S= 0.5132*R08S	Aluminum Oxide
P33E:	Water from Entrained Oxygen

IF 2.1168*R08S > 2*R12E
THEN P33E= 2*R12E
ELSE P33E= 2.1168*R08S

P41S= 2.1168*R08S-P33E	Hydrogen
P39E= R12E-0.5*P33E	Entrained Oxygen, Unreacted
P51E= R06S	Iron Oxide

Other Outputs:

Adiabatic flame temperature (K)- calculations are identical to previous models.
Fireball size and volume- calculations are identical to previous models.

b. Delta II Solids Only Model (GEM)

User definable constants:

brsa: Burn Rate of Solid propellant at 1 atmosphere pressure, meters per second
Default: brsa=0.002540
nspm: Number of Segments Per solid rocket Motor
nsia: Number of Segments Involved in the Accident
Default: nsia=1
mss: Mass of Solid propellant per Segment, grams
Default: mss= 11,702,622/nspm
awt: Average Web Thickness of the grain, meters
Default: awt=0.8

Calculations:

msia: Mass of Solids Involved in the Accident
msia= nsia * mss
gsia: Gram moles of Solid propellant Involved in the Accident
gsia= msia/46.989
Burn Time: Burn Time= awt/brsa, seconds

Reactants:	Description:
R08S= 0.27857*gsia	Ammonium Perchlorate
R07S= 0.3337*gsia	Aluminum
R09S= 0.38773*gsia	HTPB
R11E= (msia/28.84)*0.79*0.5	Nitrogen Entrained
R12E= (msia/28.84)*0.21*0.5	Oxygen Entrained

Products:

P30S= 0.0808*R08S	Carbon Dioxide
P31S= 1.2974*R08S	Carbon Monoxide
P33S= 0.7803*R08S	Water
P38S= 0.4978*R08S	Nitrogen
P43S= 0.9679*R08S	Hydrogen Chloride
P46S= 0.5739*R08S	Aluminum Oxide
P38E= R11E	Nitrogen Entrained
P33E:	Water from Entrained Oxygen
IF 1.8315*R08S > 2*R12E	
THEN P33E= 2*R12E	
ELSE P33E= 1.8315*R08S	
P41S= 1.8315*R08S-P33E	Hydrogen, Unreacted
P39E= R12E-0.5*P33E	Oxygen, Unreacted

Other Outputs:

Adiabatic flame temperature (K)- ucalculations are identical to previous models
Fireball size and volume- calculations are identical to previous models

5. Default Values of Variables and Suggested Ranges

a. Titan IV SRM

Burn rate of propellant at P = 1 atmosphere	0.002794 meters/second +/- 20%
Number of segments involved in accident	1, +99, -0.5, increments of .5
Mass of propellant per segment	2.97857E+7 grams, +/- 20%
Average web thickness of grain	1.2 meters, +/- 20%

b. Delta II GEMs

Burn rate of propellant at P = 1 atmosphere	0.00254 meters/second +/- 20%
Number of segments involved in accident	1, 1-50
Mass of propellant per segment	1.17026E+7 grams, +/- 20%
Average web thickness of grain	0.380 meters, +/- 20%

6. Test cases

Test cases for the Titan IV solids only model and the Delta II solids only model are included in Appendix F.

SECTION VI

CONCLUSIONS

The purpose of this effort was to model toxic gas releases in accidents involving the Titan II, Delta II, and Titan IV launch vehicles. Similar analyses were also performed for ground explosions involving solid rocket motor segments for the Delta II and Titan IV vehicles. This study was unique in several ways:

A. A detailed analysis of the Project Pyro tests was conducted to more accurately estimate the contribution of liquid rocket propellants to the explosive event. This contribution was important because it determined the amount of propellants thermally decomposed or released unreacted into the atmosphere. For hypergolic liquid rocket propellants (Aerozine-50 and nitrogen tetroxide), the extent of mixing and combustion during an accident was about 23 percent. For the Delta II liquid rocket propellants (RP-1 and liquid oxygen), this value was about 44 percent. Although these values were higher than previous estimates[12], significant amounts of released propellants were nonetheless predicted from on-pad or in-flight aborts of a fully loaded missile.

B. A laboratory study was performed as part of this contract; the results are included in a separate report. This study confirmed the presence of complex condensates from the mixing of solid and liquid rocket propellants. Residual nitrogen tetroxide was observed in every test in which this propellant was used and indicated incomplete combustion of this chemical. Residual Aerozine-50, on the other hand, was not observed in any test using this propellant. This result suggested that Aerozine-50 was removed from the chamber by condensation, air oxidation, thermal decomposition, or catalytic decomposition on the chamber walls. Aerozine-50 decomposition products such as ammonia, hydrogen, and methane were also absent as were the bipropellant combustion products hydrogen and carbon monoxide. The absence of these chemicals suggested afterburning with residual air. Results from the laboratory study were used in the development and modification of the source models.

C. Decomposition reactions for hydrazine, UDMH, nitrogen tetroxide, and RP-1 were reported in a variety of literature sources, and the extent of decomposition was estimated using a thermal gradient analysis of the expected combustion cloud. The estimates were consistent with results from the laboratory tests. Approximately 94 percent hydrazine, 70 percent UDMH, 70 percent RP-1, and 30 percent nitrogen tetroxide were projected to thermally decompose in an active fireball.

D. A provision was made for incorporating air entrainment into the liquid cloud source model. A variable relating the moles of air entrained to the total moles of liquid propellant available at abort was developed and used in the model. Although Project Pyro test results suggested that minimum air entrainment occurred during fireball growth and stabilization, this variable was included to provide more flexibility to the model.

E. Source models were programmed in Fortran 77 code and installed on the Cyber computer used for dispersion modeling at Vandenberg AFB, CA. Source codes were fully tested for the Titan II, Delta II, and Titan IV launch vehicles and results correlated well with those obtained from the source models. Source code listing, the Software Development File, and executable code were issued under separate cover.

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[12] An earlier Air Force working group on toxic emissions from launch vehicle explosions placed these values at about ten percent.

SECTION VII

RECOMMENDATIONS

Areas requiring further investigation are presented in the following paragraphs. These additional studies are proposed to improve the prediction of toxic chemicals arising from a launch vehicle accident. They are listed in order of priority.

A. AEROZINE-50/NITROGEN TETROXIDE MIXING

As discussed previously, the extent of reaction between Aerozine-50 and nitrogen tetroxide during an explosive event is 23 percent. These data are based on the analysis of Project Pyro tests, which are incomplete and poorly documented. Additional tests between these two propellants should be performed to evaluate the extent of mixing in a more carefully controlled manner. Data from these additional tests would provide more accurate determinations of the extent of mixing and data on statistical variations.

B. AIR ENTRAINMENT REFINEMENT

The current source models use a default value of zero for air entrainment into the liquids cloud. This value is assigned upon review of Project Pyro test data. Because the incorporation of air entrainment during fireball growth results in atmospheric burning of residual fuels (Aerozine-50 and RP-1), a more detailed investigation into the extent of air entrainment should be undertaken.

C. SOFTWARE VALIDATION

Software developed under this effort is engineering development software, and as such is not intended to support flight operations. Although the software has been fully tested[13], more rigorous testing and evaluation should be performed to upgrade this software for operational use.

D. HEAT FLUX MEASUREMENTS

Source models and software programs do not incorporate heat flux equations. The incorporation of these thermal decay mechanisms would allow for more accurate modeling of the accident thermal environments and should be incorporated into future source models and software programs.

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[13]Six test cases, corresponding to the the conditions identified in Tables 16,22,23,29, and 30 were executed on the developed Fortran 77 computer program. Results from these computer runs correlated well with results obtained from the analytical models.

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APPENDIX A

HEAT FLUX CALCULATIONS, CONTINUED BURNING REACTIONS

A. RP-1/LOX ENERGY RELEASE FROM PROJECT PYRO 25,000 POUND TEST

$W := 25000$ — **total weight of propellants,lb** (A-1)

$to := 0.196 \cdot W^{.349}$ — **Fireball Duration, sec.** (A-2)

$A := 4 \cdot \pi \cdot 335^{2}$ — **Area of sphere where radiant heat flux measurements were taken** (A-3)

$$q(t) := \left[501.97 \cdot \left(\frac{t}{to}\right)^{7} - 1964.35 \cdot \left(\frac{t}{to}\right)^{6} + 3131.92 \cdot \left(\frac{t}{to}\right)^{5} - 2610.56 \cdot \left(\frac{t}{to}\right)^{4} + 1211.1 \cdot \left(\frac{t}{to}\right)^{3} - 307.114 \cdot \left(\frac{t}{to}\right)^{2} + 37.321 \cdot \left(\frac{t}{to}\right) + .064\right] \cdot .88125$$

Thermal radiation from a LOX/RP-1 fireball, curve fit from MEAN PYRO data, BTU/sec*Ft^2 (A-4)

$$Q := \int_{0}^{to} q(t)\, dt \cdot A$$

Integrate fireball area times heat flux per unit area from t=0 to t=to (A-5)

$Q = 9.413 \cdot 10^{6}$ — **TOTAL HEAT RADIATED DURING ACTIVE BURNING PHASE OF A LOX/RP-1 FIREBALL, BTU's.** (A-6)

CHECK NUMBERS AT THE BOUNDRY CONDITIONS- DO THEY MAKE SENSE?

$to = 6.716$ $\quad q(to) = 0.309$ $\quad q(0) = 0.056$ $\quad A = 1.41 \cdot 10^{6}$

$cp := 0.460$ — **average Heat capacity of fireball gases BTU/lb. R** (A-7)

$T := 3316 - 460$ — **overall Temperature rise of fireball, R (Final fireball temp. was determined using the same Mean Raidant Heat flux data)** (A-8)

Added Enthalpy of fireball at burnout, BTU (A-9)

$Qfb := W \cdot cp \cdot T$ — **"" "" "" ""**

$Qfb = 3.284 \cdot 10^{7}$

$Hv := .183 \cdot 12500 + 106 \cdot 12500$ — **Enthalpy of vaporization of the propellants, BTU** (A-10)

$Hv = 1.327 \cdot 10^{6}$ — **"" "" "" ""**

$QT := Q + Qfb + Hv$ — **Total enthalpy released during reaction.BTU** (A-11)

$QT = 4.358 \cdot 10^{7}$ — **"" "" "" ""**

Heat of reaction, BTU/lb.(RP-1) (A-12)

$Hr := 7870.6$

Mass of RP-1, lb. (A-13)

$mRP1 := 12500$

Total chemical energy avail. in initial propellant mass, BTU

$Qmax := mRP1 \cdot Hr$ — **" " " " "**

$Qmax = 9.838 \cdot 10^{7}$ (A-14)

Percent of initial propellant mass reacted.

$$PercentReacted := \left(\frac{QT}{Qmax}\right) \cdot 100 \qquad \text{(A-15)}$$

$PercentReacted = 44.3$

B. A-50/N_2O_4 ENERGY RELEASE FROM PROJECT PYRO 1,000 POUND TEST

$W := 1000$ **weight of propellant** (A-16)

$to := .196 \cdot W^{.349}$ **fireball duration** (A-17)

$$Y(t) := -8.93413 \cdot 10^{8} \cdot \left(\frac{t}{to}\right)^{5} + 8.06087 \cdot 10^{7} \cdot \left(\frac{t}{to}\right)^{4} + 295856 \cdot \left(\frac{t}{to}\right)^{3} - 223999 \cdot \left(\frac{t}{to}\right)^{2} + 6552.75 \cdot \left(\frac{t}{to}\right) + 1.16313 \qquad \text{(A-18)}$$

CURVE FIT FOR MEAN HEAT FLUX DATA- INITIAL PULSE

$Q := \int_{0}^{.055} Y(t)\,dt$ **integrate initial pulse curve from to=0 to to=.055** (A-19)

$Q = 2.336$ **total heat resulting from the initial heat flux pulse** (A-20)

$$Z(t) := 197738 \cdot \left(\frac{t}{to}\right)^{8} - 895028 \cdot \left(\frac{t}{to}\right)^{7} + 1.68502 \cdot 10^{6} \cdot \left(\frac{t}{to}\right)^{6} - 1.70584 \cdot 10^{6} \cdot \left(\frac{t}{to}\right)^{5} + 1.00264 \cdot 10^{6} \cdot \left(\frac{t}{to}\right)^{4} - 344804 \cdot \left(\frac{t}{to}\right)^{3} + 66385 \cdot \left(\frac{t}{to}\right)^{2} - 6371.67 \cdot \left(\frac{t}{to}\right) + 261.522 \qquad \text{(A-21)}$$

CURVE FIT FOR MEAN HEAT FLUX DATA- CONTINUED BURNING

$q := \int_{.056}^{1} Z(t)\,dt$ **integrate continued burning heat flux from to=.056 to to=1** (A-22)

$q = 37.16$ **total heat resulting from the continued burning** (A-23)

$multiplier = \frac{q}{Q}$ (A-24)

$multiplier = 15.906$

APPENDIX B

LIQUID ROCKET PROPELLANT AIR ENTRAINMENT

One of the more difficult problems associated with the description of a rocket propellant fireball is defining the extent of air entrained during the active burning phase. No empirical data are available to define this phenomena, so the required information must be inferred from other types of data.

From Project Pyro and other large scale propellant tests, the fireball volume reported at burnout exceeds volumes calculated using the combustion products and unreacted propellants at the measured fireball temperatures. This calculation assumes the fireball internal pressure equilibrates with atmospheric pressure, and that the ideal gas law applies. On the other hand, thermal and plume rise/buoyancy data from these tests indicate negligible air entrainment into the fireball.

Based upon this conflicting data, the extent of air entrainment into an actively burning fireball cannot be readily determined. The uncertainty of the volume measurements, estimated at plus or minus 30 percent, in conjunction with the unknown fireball internal pressure at burnout, produces uncertainty in the use of fireball volumes as a measure of air entrainment. Thermal data from Project Pyro tests are more reliable and repeatable and provide improved estimates of air entrainment. In addition, the overpressure shock wave emitted during the initial explosive mixing event would expel the surrounding air away from the mixed and vaporized propellants at the fireball center, and leave a vacuum into which the fireball could expand. Although the expansion process is turbulent, negligible air is available in the immediate vicinity of the expanding fireball. For these reasons, the assumption was made that no air is entrained into an actively growing liquid propellant fireball.

If future data or analysis indicate significant air entrainment into a liquid propellant fireball, an option to incorporate entrained air into the source models and Fortran 77 code is provided. Air entrainment calculations are based on the following assumptions.

A. Since the fireball consists of a fuel cell (in which fuel decomposition products are contained) and an oxidizer cell, the air is entrained into the fireball cells equally, on a molar basis.

B. The air entrained into the oxidizer cell dilutes and cools the cell. No reactions between the air and the oxidizer are expected.

C. The oxygen entrained into the fuel cell reacts with unreacted fuels and fuel decomposition products. The nitrogen entrained into the fuel cell dilutes and cools the cell.

D. For an Aerozine-50 cell, the oxygen entrained into the cell reacts equally with the UDMH and the N_2H_4 on a molar basis until the oxygen is depleted. One molecule of hydrazine burns with one molecule of UDMH. The stoichiometries of these reactions are:

$$N_2H_4 + O_2 \rightarrow N_2 + 2\,H_2O \qquad \text{(B-1)}$$

$$C_2H_8N_2 + 4\,O_2 \rightarrow 2\,CO_2 + 4\,H_2O + N_2 \qquad \text{(B-2)}$$

For every five molecules of oxygen entrained into an Aerozine-50 cell, four molecules of oxygen react with UDMH and one molecule reacts with hydrazine.

E. For an RP-1 cell, all oxygen entrained into the cell reacts with RP-1 until the oxygen or the RP-1 is depleted. The stoichiometry is identical to that used for LOX/RP-1.

APPENDIX C

DELTA II SOLID ROCKET PROPELLANT AIR ENTRAINMENT

This analysis was based upon the GEMs breakup analysis performed by the Research Triangle Institute (RTI). The fragmentation data from this report were used to determine the average fragment size and number for both the ground ignited (GI) and the air ignited (AI) solid rocket motors. The following assumptions were used to develop this model.

A. All AI motors are fragmented and ignited by either the exploding core vehicle, or the destruct package.

B. The propellant fragments are cubic in shape and burn on all six sides.

C. All burning fragments are the mean size based upon initial burning surface area.

D. The average fragment initial vertical velocity is zero. The forward velocity of the vehicle prior to accident was not considered in the model.

E. The fragments burning while falling through the air will entrain 100 percent air by volume instantaneously due to the turbulence.

F. The fragments burning on the ground will entrain 50 percent by volume prior to burnout.

G. Fragment terminal velocity is 200 feet per second.

H. The burn rate of the propellant at one atmosphere pressure is 0.10 inches per second. This is derived from the burn rate equation[14] for the propellant at elevated pressures and applied at one atmosphere. The following steps were taken to develop the model.

1. Curve fits of the RTI data were generated for the number, surface area, and size of the propellant fragments as a function of abort time in seconds.

2. A series of equations were developed which defined the pounds of propellant burned in air and on the ground as a function of the time and elevation of the abort.

3. The model was segregated into three distinct phases.

a. 0-615 feet. For aborts in this elevation range, the fragments continually accelerate until they impact the ground.

b. 616-5800 feet. The fragments reach terminal velocity before hitting the ground, and both GI and AI motor fragments impact the ground and continue to burn there.

c. 5801-10000 feet. The GI motor fragments burn out before impacting the ground, and the AI motor fragments reach the ground and continue to burn there.

The following pages present the curve fits and mathematical model generated.

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[14]The burn rate equation takes the form $r = aP^n$, where r is the propellant burn rate expressed in inches per second, P is the pressure in pounds per square inch, a is an empirical constant, and n is the burning rate pressure exponent.

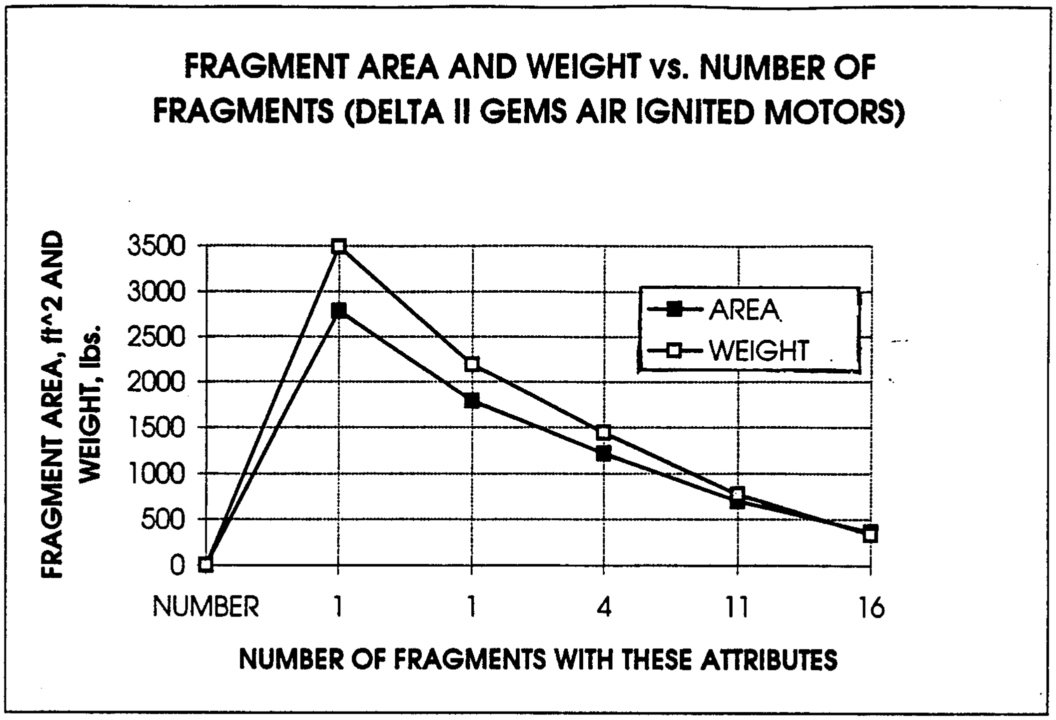

Figure C-1. RTI Fragmentation Data, GEMs Air Ignited Motors.

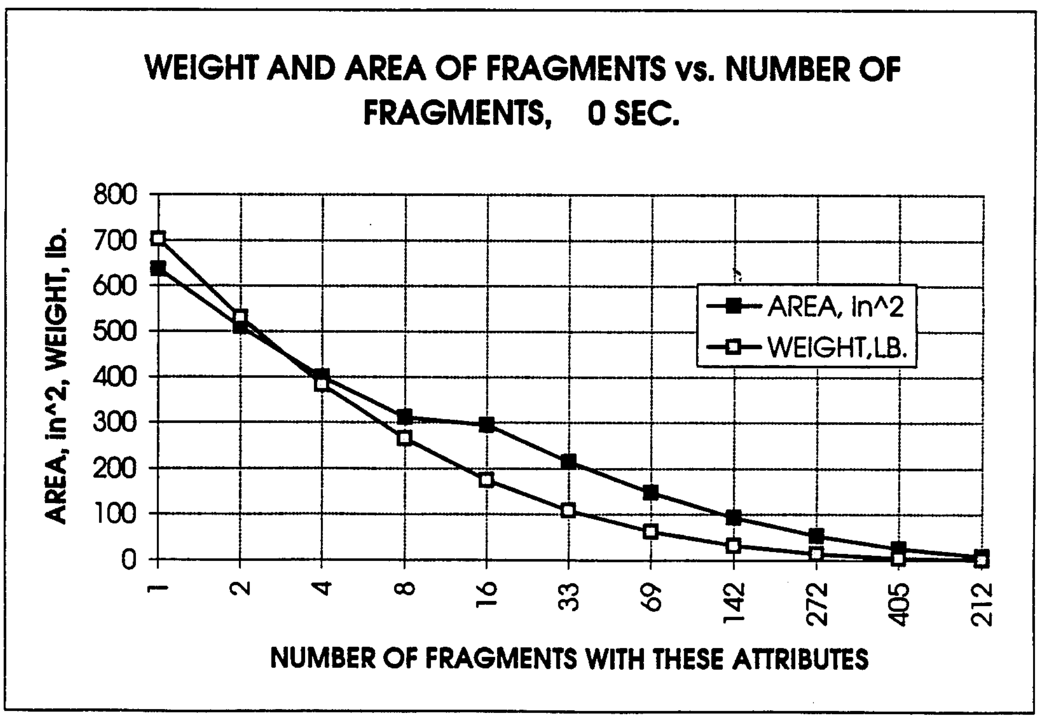

Figure C-2. RTI Fragmentation Data, 0 Seconds.

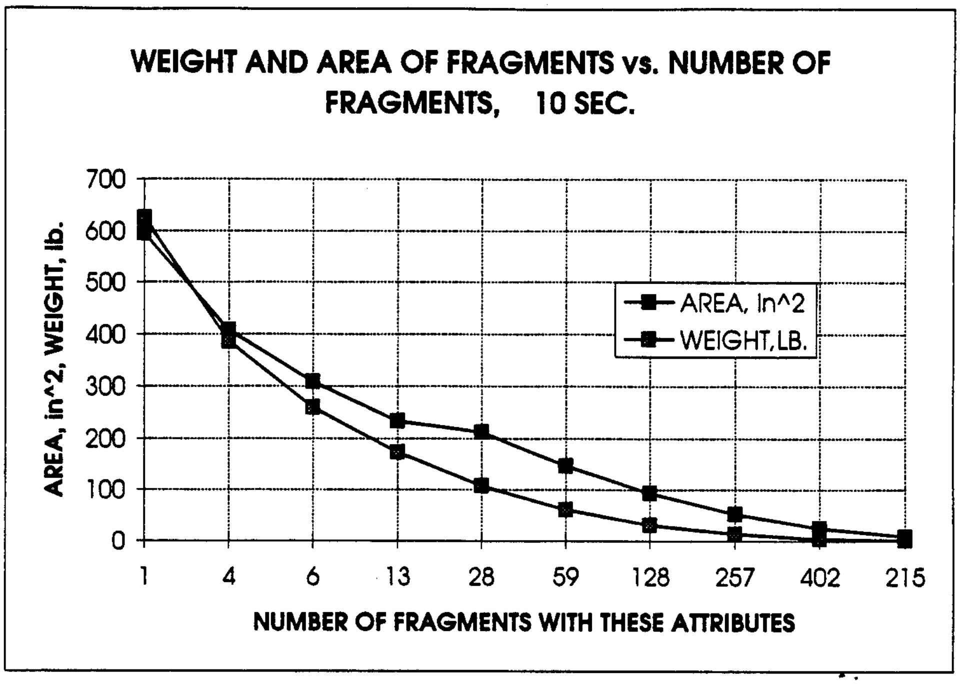

Figure C-3. RTI Fragmentation Data, 10 Seconds.

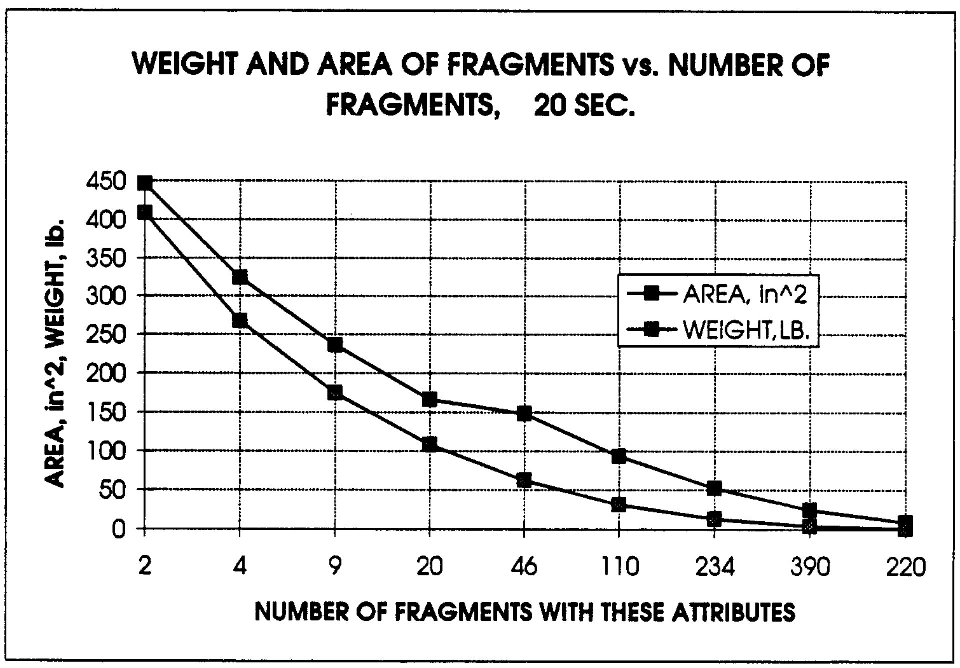

Figure C-4. RTI Fragmentation Data, 20 Seconds.

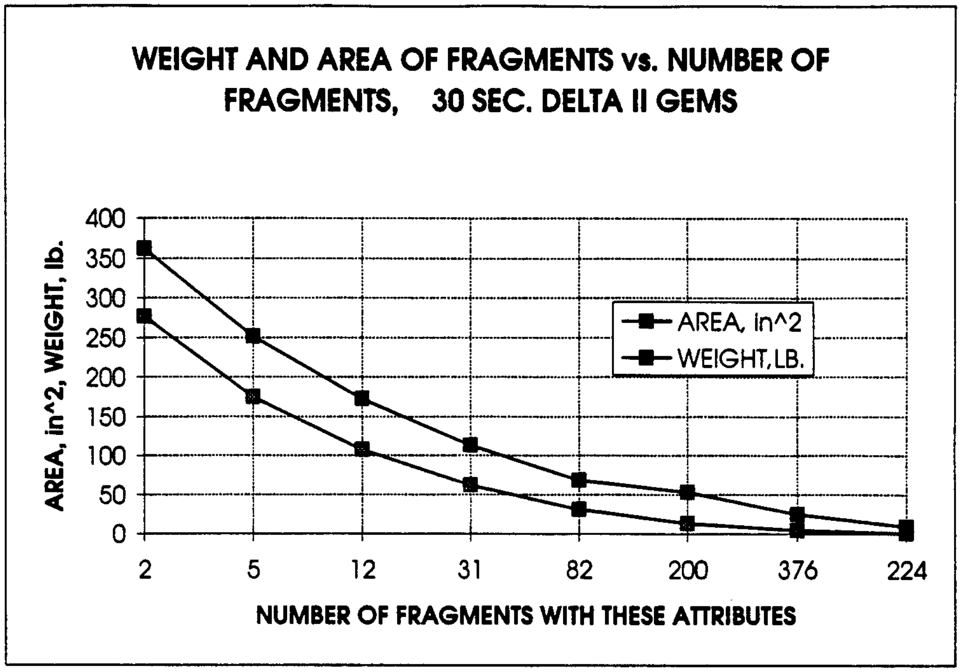

Figure C-5. RTI Fragmentation Data, 30 Seconds.

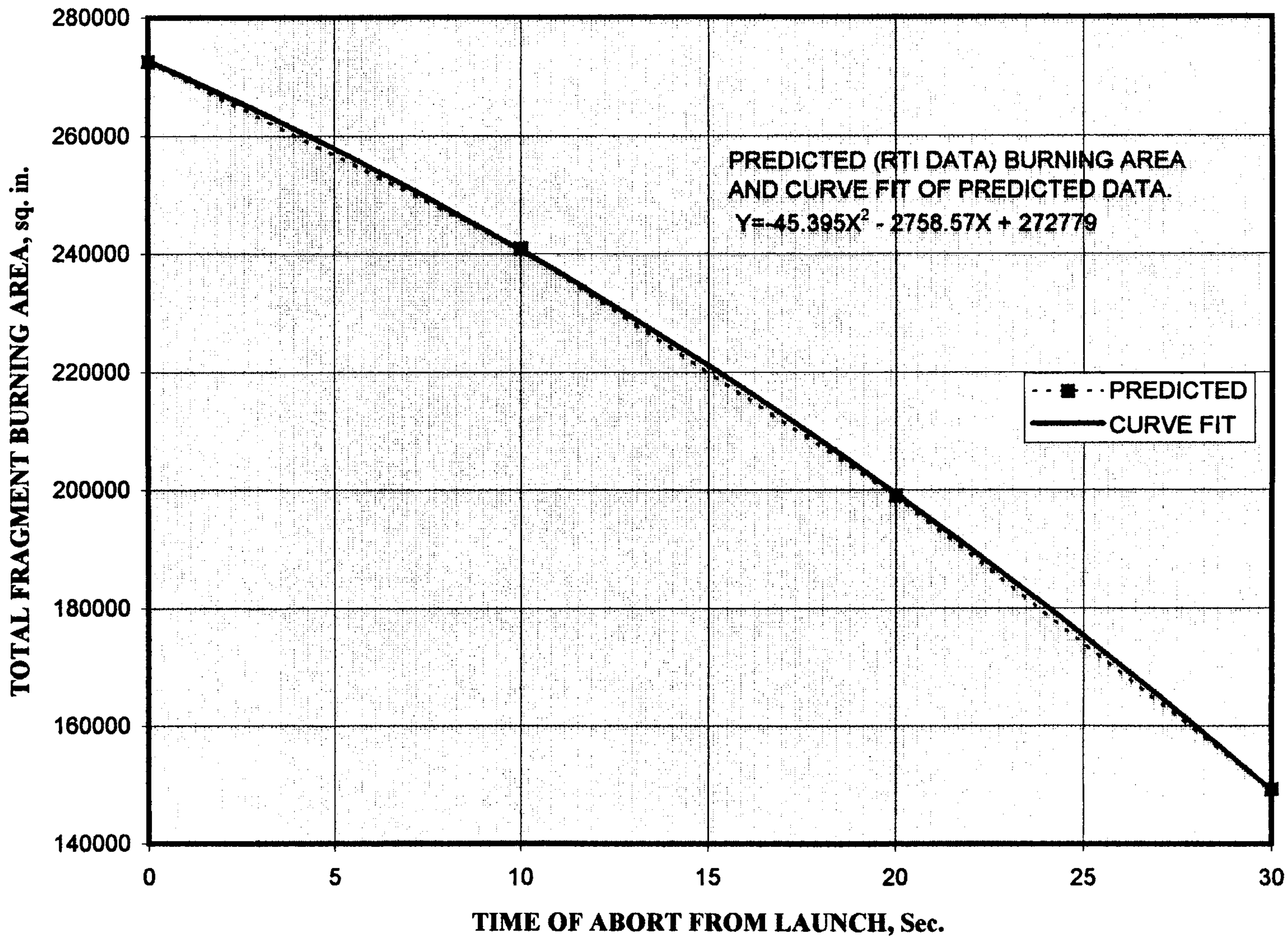

Figure C-6. Total Fragment Surface Area vs Time from Normal Ignition.

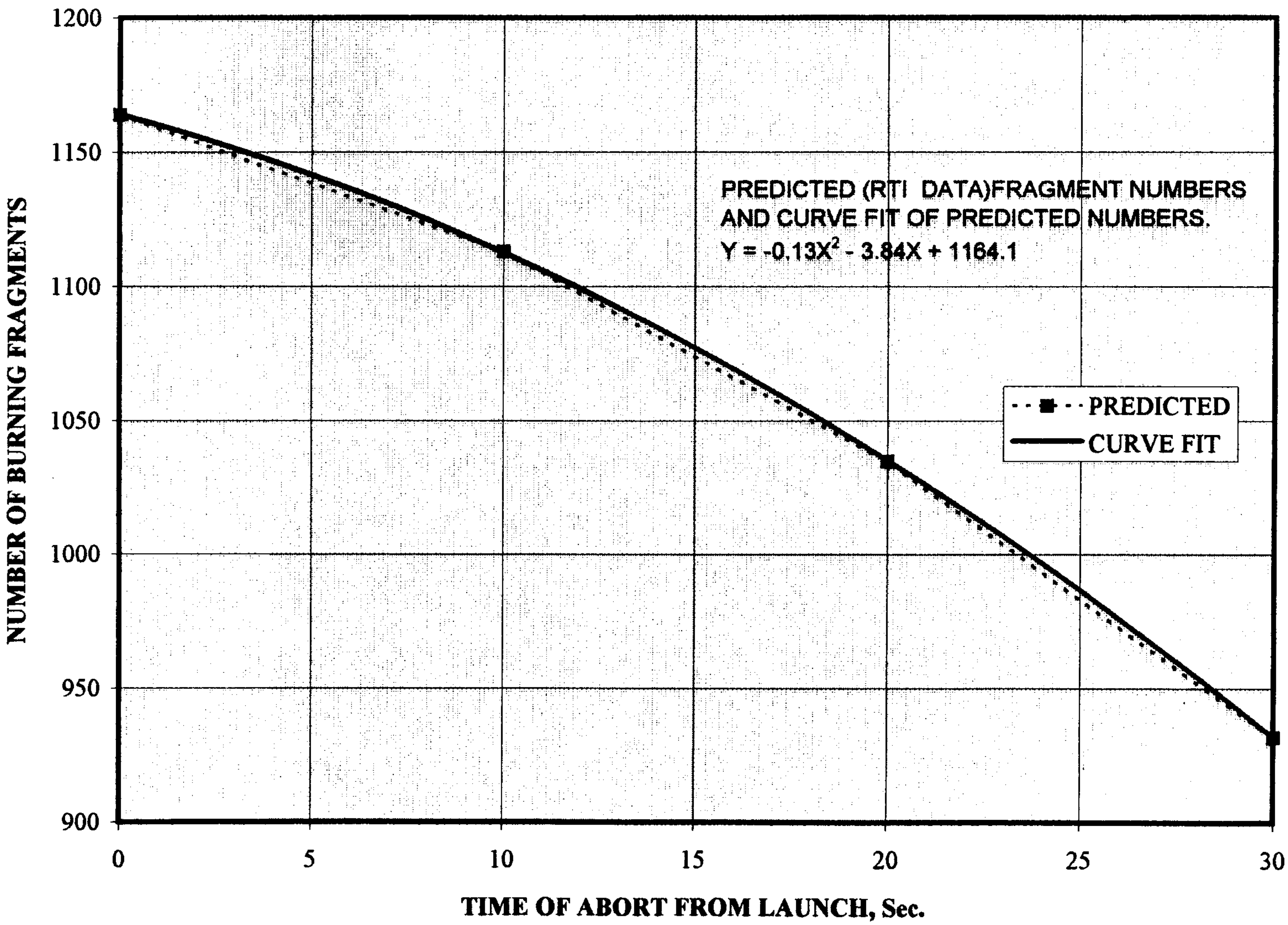

Figure C-7. Number of Fragments vs Time of Abort.

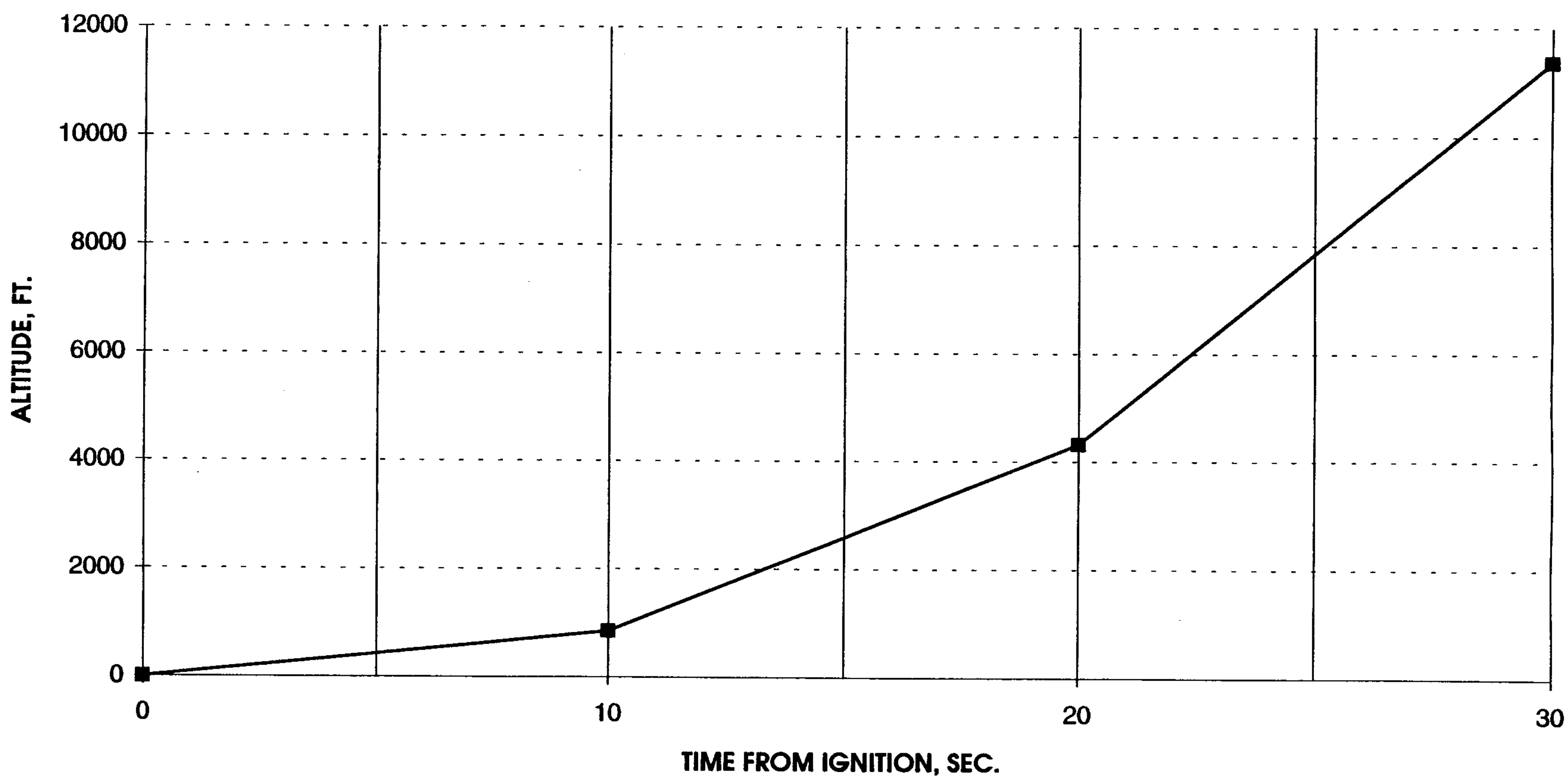

Figure C-8. Trajectory, Delta II GEMs.

DELTA II GEMS FRAGMENTATION AND BURNING FOR ABORTS BELOW 615 FEET ALTITUDE

$n := 0..62$ **ITERATOR** (C-1)

$a_n := 10 \cdot n$ **ELEVATION OF ABORT, FT.** (C-2)

$s_n := \frac{6.5}{62} \cdot n$ **TIME OF ABORT, SEC. AFTER IGNITION** (C-3)

$FWA(s) := \frac{25800 - 395 \cdot s_n}{\left[-0.13 \cdot (s_n)^2 - 3.84 \cdot s_n + 1164.1\right]}$ **FRAGMENT WEIGHT AT ABORT (GI, LB)** (C-4)

$FLA(s) := \left(\frac{FWA(s)}{0.06366}\right)^{\frac{1}{3}}$ **FRAGMENT CUBE EDGE DIMENSION (GI, IN.)** (C-5)

$FNA(s) := -0.13 \cdot (s_n)^2 - 3.84 \cdot s_n + 1164.1$ **NUMBER OF FRAGMENTS (GI, LB)** (C-6)

$FTA(a) := \sqrt{\frac{2 \cdot a_n}{32}}$ **FRAGMENT TIME FALLING THROUGH AIR (GI & AI, SEC)** (C-7)

$FBAGI_n := \left[\left[FLA(s)^3 - (FLA(s) - 0.2 \cdot FTA(a))^3\right] \cdot 0.06366\right] \cdot 6 \cdot FNA(s)$ **LB. GI FRAGMENTS BURNED WHILE FALLING** (C-8)

$FBAAI_n := \left[\left[10662.5266 - (22.01 - 0.2 \cdot FTA(a))^3\right] \cdot 0.06366\right] \cdot 38 \cdot 3$ **LB. AI FRAGMENTS BURNED WHILE FALLING** (C-9)

$FBA := FBAAI + FBAGI$ **TOTAL MASS OF PROPELLANT BURNED WHILE FALLING** (C-10)

$FBG_n := \left[(25800 - 395 \cdot s_n) \cdot 6 - FBAGI_n\right] + \left[(3 \cdot 25800) - FBAAI_n\right]$ **TOTAL MASS OF PROPELLANT BURNING ON THE GROUND** (C-11)

$WPT_n := FBAGI_n + FBAAI_n + FBG_n + (395 \cdot s_n \cdot 6)$ **CHECK THAT TOTAL MASS OF PROPELLANT IS ACCOUNTED FOR AT ALL TIMES** (C-12)

$AE(a) := (FNA(s) \cdot a_n \cdot .0332 + 114.2513 \cdot a_n + 0.5 \cdot FBG_n) \cdot .946$ **AIR ENTRAINED INTO SOLIDS CLOUD** (C-13)

FBA=TOTAL MASS OF PROPELLANT BURNED WHILE FALLING
FBAAI=AIR IGNITED MOTOR CONTRIBUTION
FBAGI=GROUND IGNITED MOTOR CONTRIBUTION

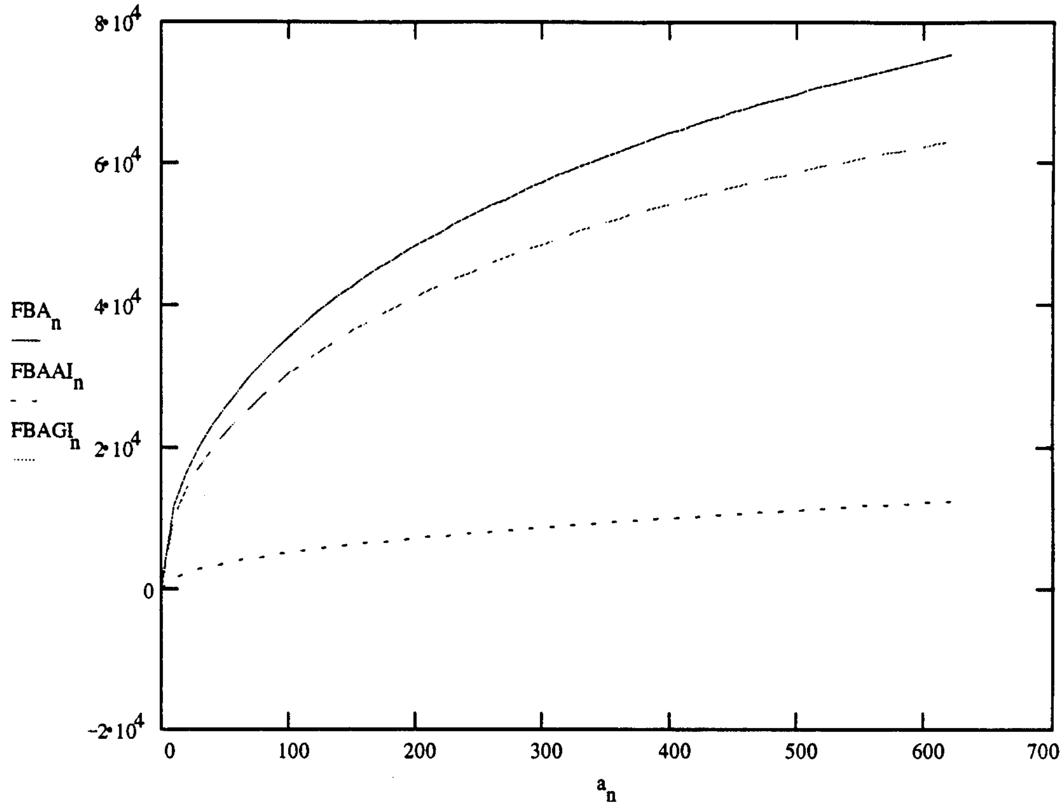

Figure C-9. Total Propellant Mass Burned During Descent (Altitude < 615 Feet).

FLA=FRAG. CUBE EDGE LENGTH

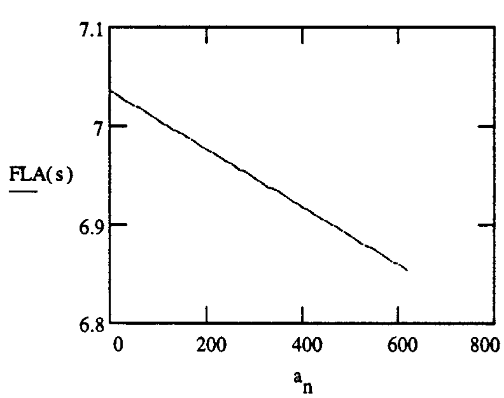

Figure C-10. GEMs Fragment Cube Edge Length (Altitude < 615 Feet).

FWA=FRAG. WEIGHT AT ABORT

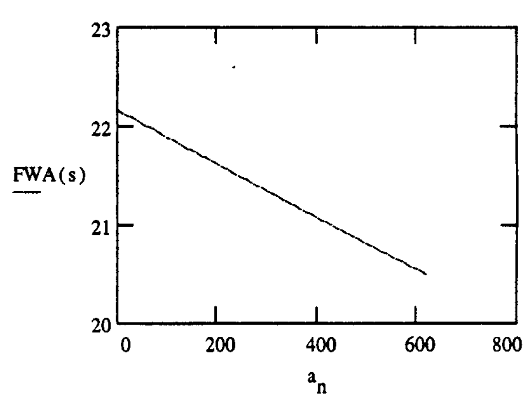

Figure C-11. GEMs Fragment Weight (Altitude < 615 Feet).

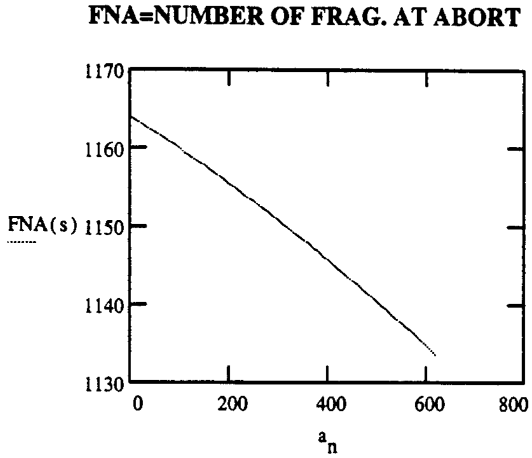

Figure C-12. Number of GEMs Fragments (Altitude < 615 Feet).

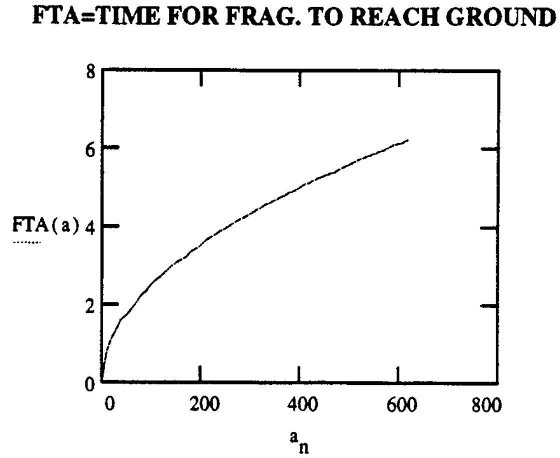

Figure C-13. GEMs Descent Time (Altitude < 615 Feet).

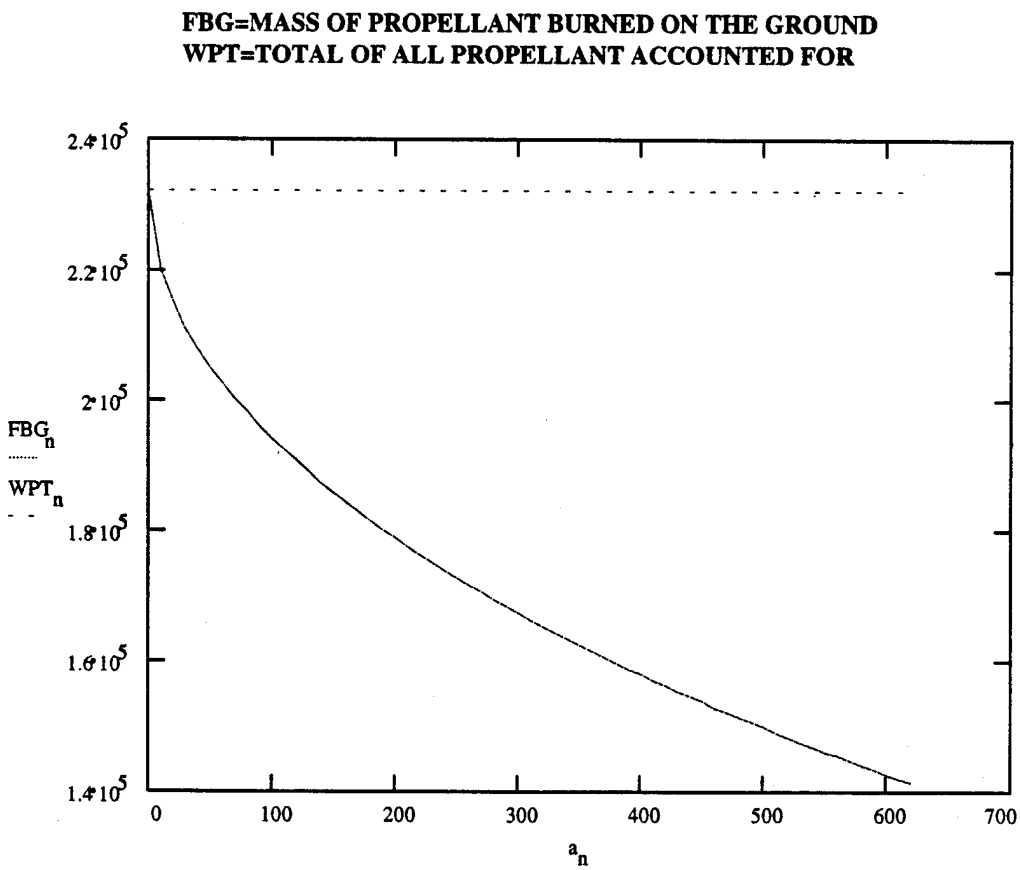

Figure C-14. Total GEMS Propellant Mass Burned on the Ground (Altitude < 615 Feet).

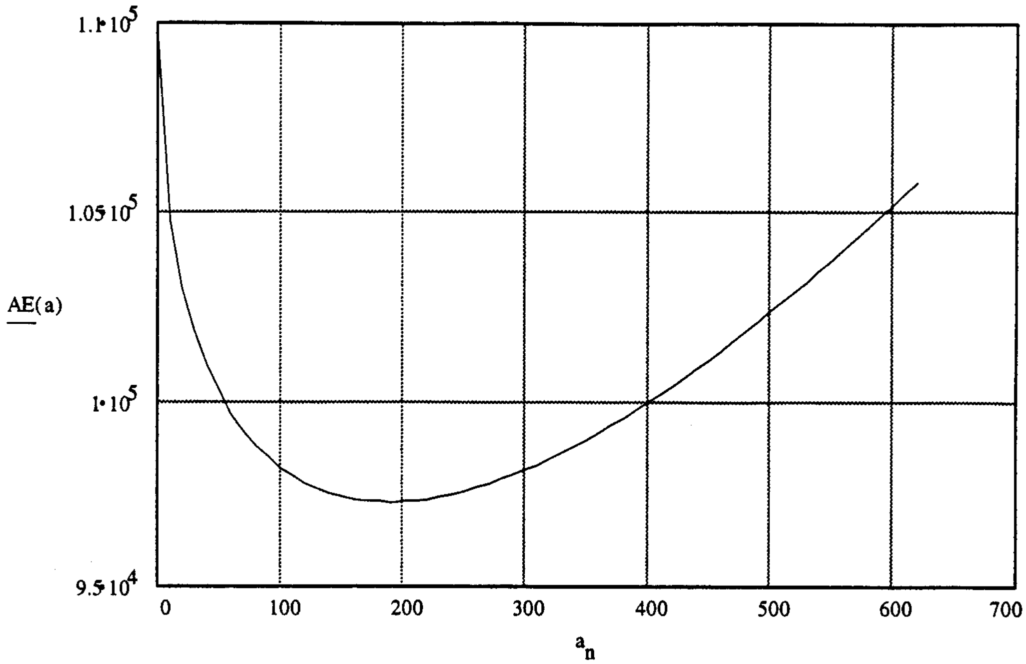

Figure C-15. GEMS Air Entrainment as a Function of Elevation (Altitude < 615 Feet).

DELTA II GEMS FRAGMENTATION AND BURNING FOR ABORTS FROM 615 TO 5800 FEET ALTITUDE

$n := 1..51$ (C-14)

$a_n := 700 + 100 \cdot n$ **ELEVATION OF ABORT, FT.** (C-15)

$s_n := 6.5 + \left(\frac{28}{93}\right) \cdot n$ **TIME OF ABORT, SEC. AFTER IGNITION** (C-16)

$FWA(s) := \frac{25800 - 395 \cdot s_n}{\left[-0.13 \cdot (s_n)^2 - 3.84 \cdot s_n + 1164.1\right]}$ **FRAGMENT WEIGHT AT ABORT (GI, LB)** (C-17)

$FLA(s) := \left(\frac{FWA(s)}{0.06366}\right)^{\frac{1}{3}}$ **FRAGMENT CUBE EDGE DIMENSION (GI, IN.) AT ABORT** (C-18)

$FNA(s) := -0.13 \cdot (s_n)^2 - 3.84 \cdot s_n + 1164.1$ **NUMBER OF FRAGMENTS AT ABORT (GI, LB)** (C-19)

$FTA(a) := 6.2 + \frac{a_n - 615}{200}$ **FRAGMENT TIME FALLING THROUGH AIR (GI & AI, SEC)** (C-20)

$FLAGI(a) := FLA(s) - 0.2 \cdot FTA(a)$ **FRAGMENT CUBE SIDE LENGTH AT GROUND IMPACT, IN.** (C-21)

$FBAGI_n := \left[\left[FLA(s)^3 - (FLA(s) - 0.2 \cdot FTA(a))^3\right] \cdot 0.06366\right] \cdot 6 \cdot FNA(s)$ **LB. GI FRAGMENTS BURNED** (C-22)

$FBAAI_n := \left[\left[10662.5266 - (22.01 - 0.2 \cdot FTA(a))^3\right] \cdot 0.06366\right] \cdot 38 \cdot 3$ **LB. AI FRAGMENTS BURNED FALLING** (C-23)

$FBA := FBAAI + FBAGI$ **TOTAL MASS OF PROPELLANT BURNED WHILE FALLING** (C-24)

$FBG_n := \left[(25800 - 395 \cdot s_n) \cdot 6 - FBAGI_n\right] + \left[(3 \cdot 25800) - FBAAI_n\right]$ **TOTAL MASS OF PROPELLANT BURNING ON THE GROUND** (C-25)

$WPT_n := FBAGI_n + FBAAI_n + FBG_n + (395 \cdot s_n \cdot 6)$ **CHECK THAT TOTAL MASS OF PROPELLANT IS ACCOUNTED FOR AT ALL TIMES** (C-26)

$AE(a) := \left[(FNA(s) \cdot a_n \cdot .0332) + (114 \cdot .2513 \cdot a_n) + .5 \cdot FBG_n\right] \cdot .946$ **AIR ENTRAINED BY SOLIDS CLOUD** (C-27)

FBA=TOTAL MASS OF PROPELLANT BURNED WHILE FALLING
FBAAI=AIR IGNITED MOTOR CONTRIBUTION
FBAGI=GROUND IGNITED MOTOR CONTRIBUTION
FBG=MASS OF PROPELLANT BURNED ON GROUND
WPT=TOTAL MASS OF PROPELLANT ACCOUNTED FOR

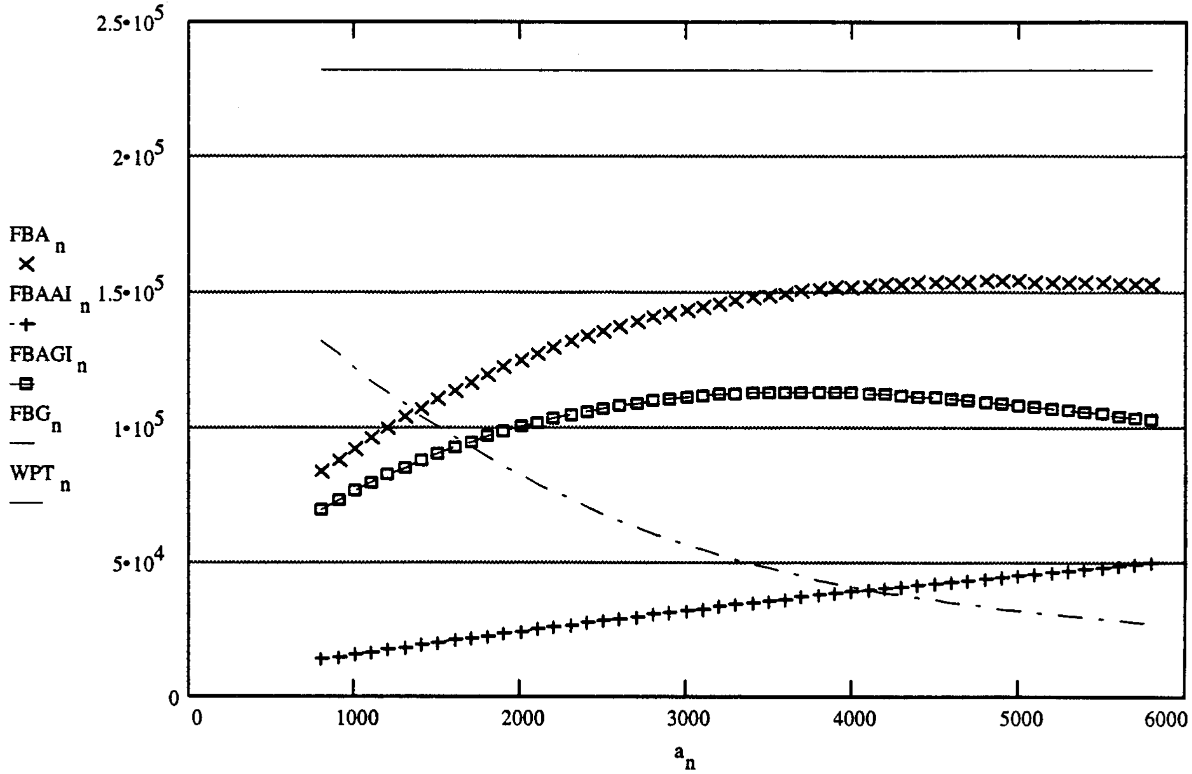

Figure C-16. Total Mass of GEMs Propellant Burned (615-5800 Feet Altitude).

FLA=FRAG. CUBE EDGE LENGTH

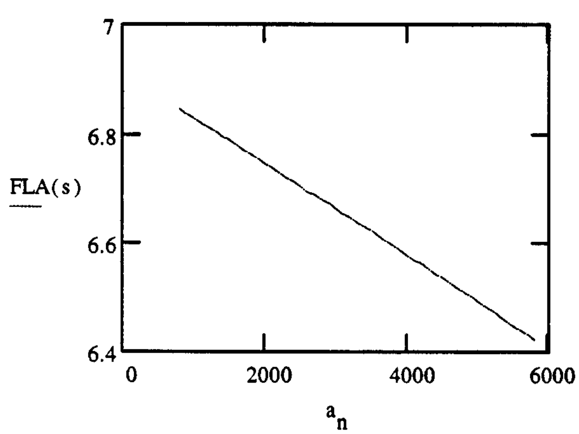

Figure C-17. GEMs Fragment Cube Edge Length (615-5800 Feet Altitude).

FWA=FRAG. WEIGHT AT ABORT

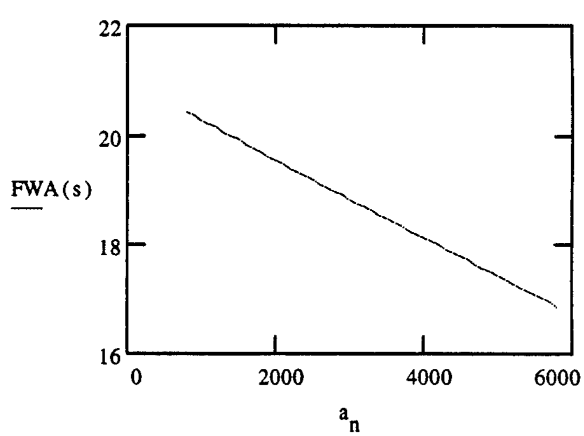

Figure C-18. GEMs Fragment Weight (615-5800 Feet Altitude).

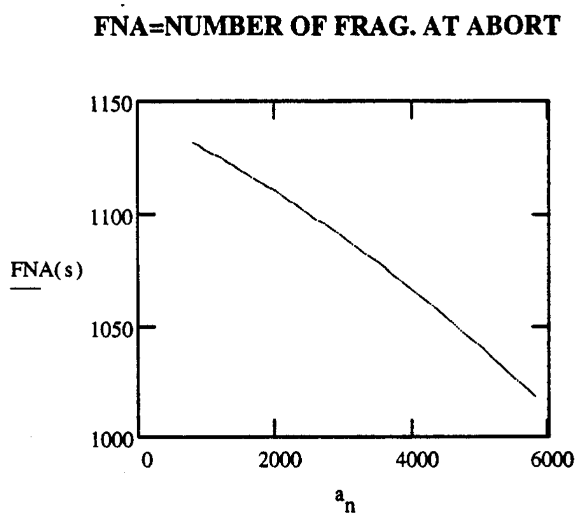

Figure C-19. Number of GEMs Fragments (615-5800 Feet Altitude).

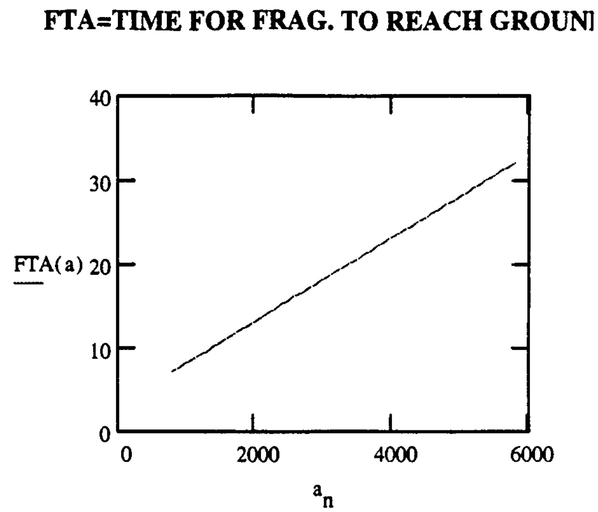

Figure C-20. GEMs Descent Time (615-5800 Feet Altitude).

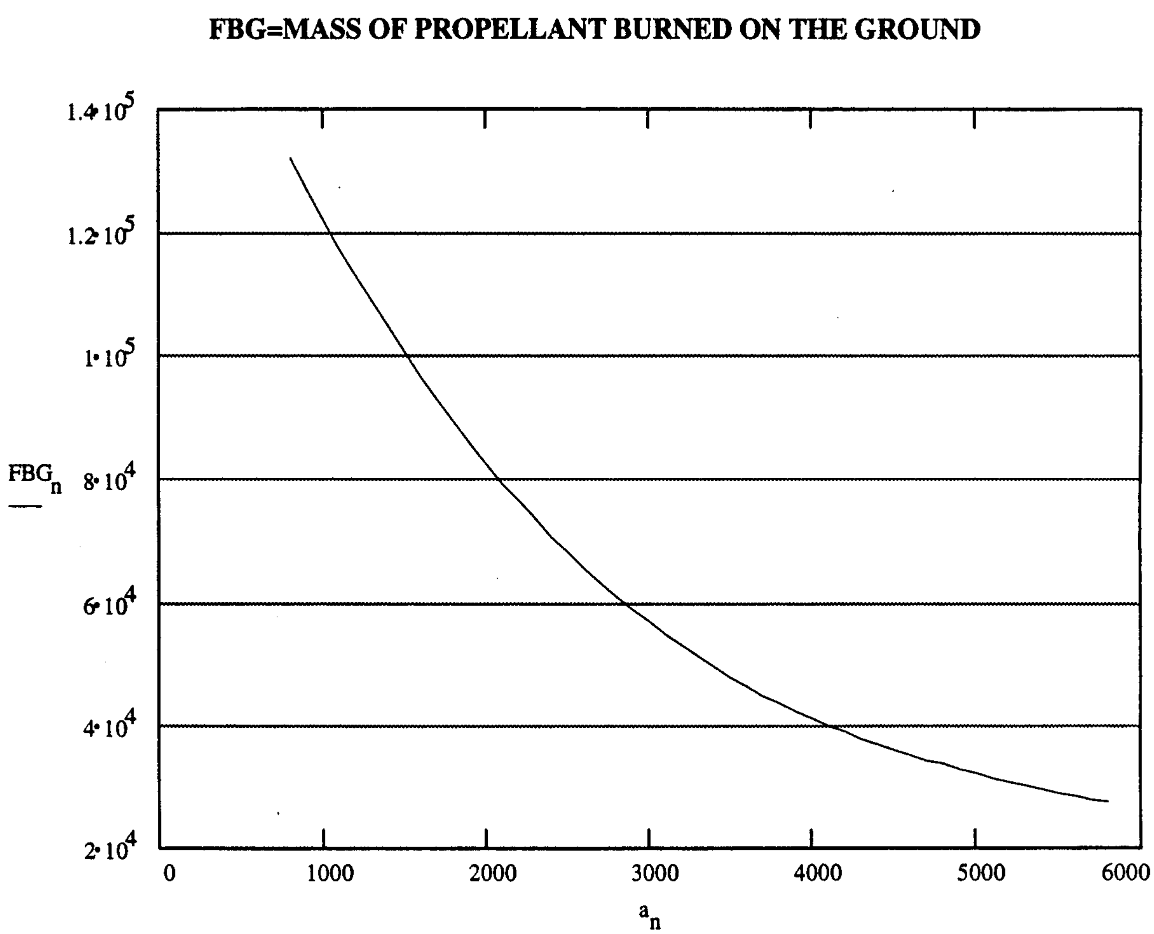

Figure C-21. Total GEMs Propellant Mass Burned on the Ground (615-5800 Feet Altitude).

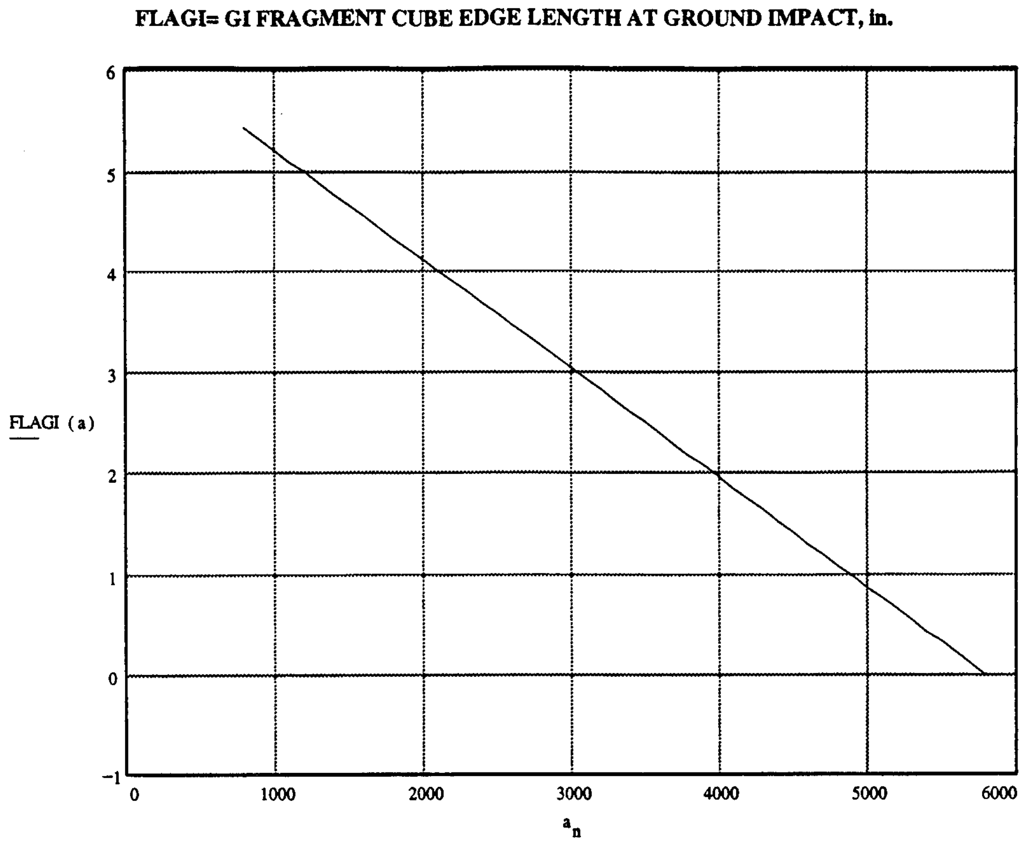

Figure C-22. GEMS Cube Edge Length at Ground Impact (615-5800 Feet Altitude).

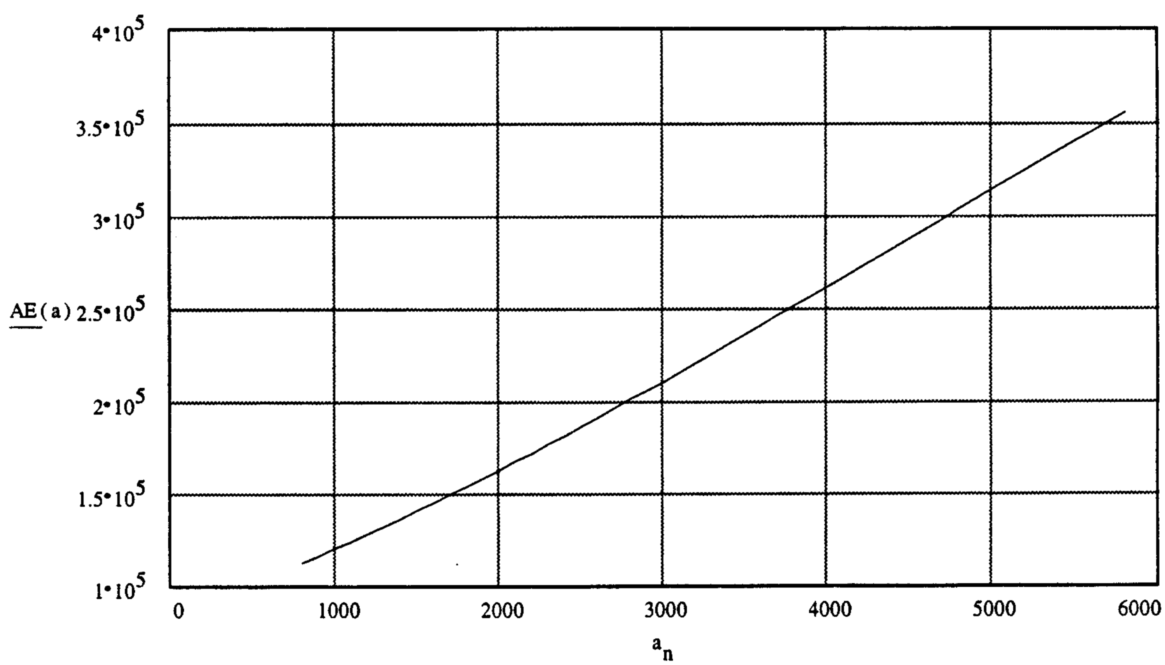

Figure C-23. Mass of Air Entrained, GEMs (615-5800 Feet Altitude).

DELTA II GEMS FRAGMENTATION AND BURNING FOR ABORTS ABOVE 5800 FEET ALTITUDE

$n := 51 .. 93$ (C-28)

$a_n := 700 + 100 \cdot n$ **ELEVATION OF ABORT, FT.** (C-29)

$s_n := 6.5 + \left(\frac{28}{93}\right) \cdot n$ **TIME OF ABORT, SEC. AFTER IGNITION** (C-30)

$FTA(a) := 6.2 + \frac{a_n - 615}{200}$ **FRAGMENT TIME FALLING THROUGH AIR (AI, SEC)** (C-31)

$FBAAI_n := \left[\left[10662.5266 - (22.01 - 0.2 \cdot FTA(a))^3\right] \cdot 0.06366\right] \cdot 38 \cdot 3$ **LB. AI FRAGMENTS BURNED FALLING** (C-32)

$FBA := FBAAI$ **TOTAL MASS OF PROPELLANT BURNED WHILI FALLING** (C-33)

$FBG_n := \left[(3 \cdot 25800) - FBAAI_n\right]$ **TOTAL MASS OF PROPELLANT BURNING ON THE GROUND** (C-34)

$WPT_n := 6 \cdot 25800 + FBAAI_n + FBG_n$ **CHECK THAT TOTAL MASS OF PROPELLANT IS ACCOUNTED FOR AT ALL TIMES** (C-35)

$AE(a) := \left[(954.66 \cdot 5800 \cdot 0.0332) + \left(114 \cdot 0.2513 \cdot a_n\right) + 0.5 \cdot FBG_n\right] \cdot 0.946$ **AIR ENTRAINED BY SOLIDS COMBUSTION PRODUCT CLOUD** (C-36)

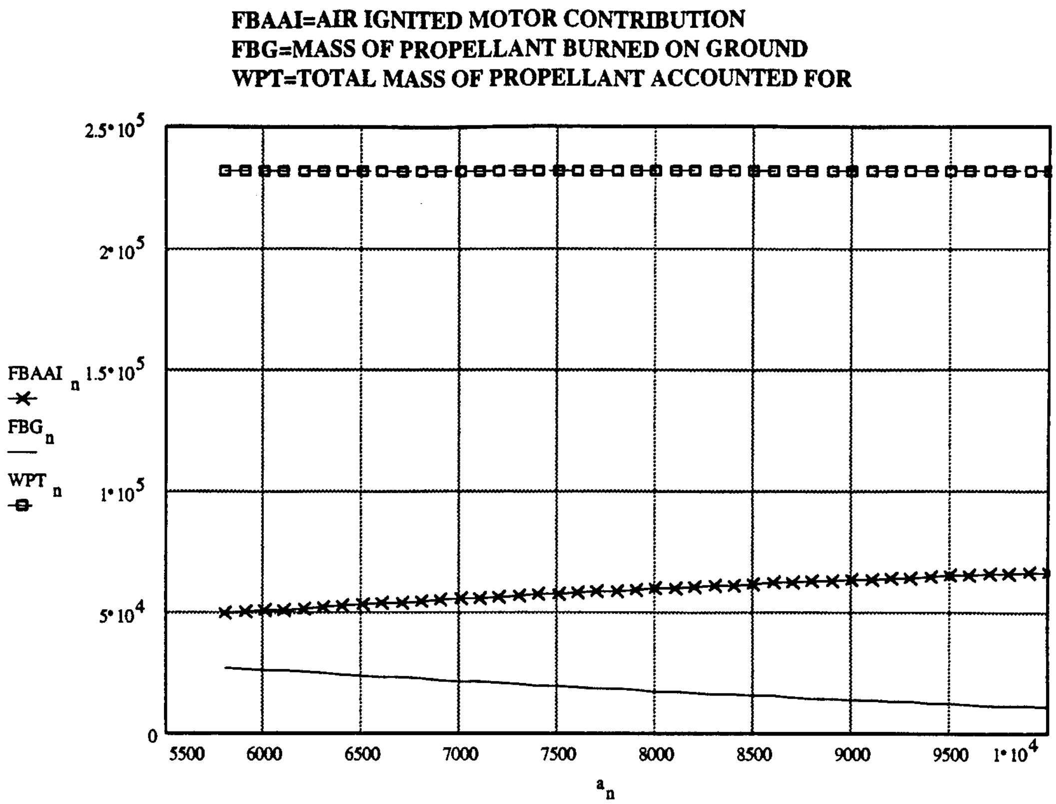

Figure C-24. Total Mass of GEMs Propellant Burned (Altitude > 5800 Feet).

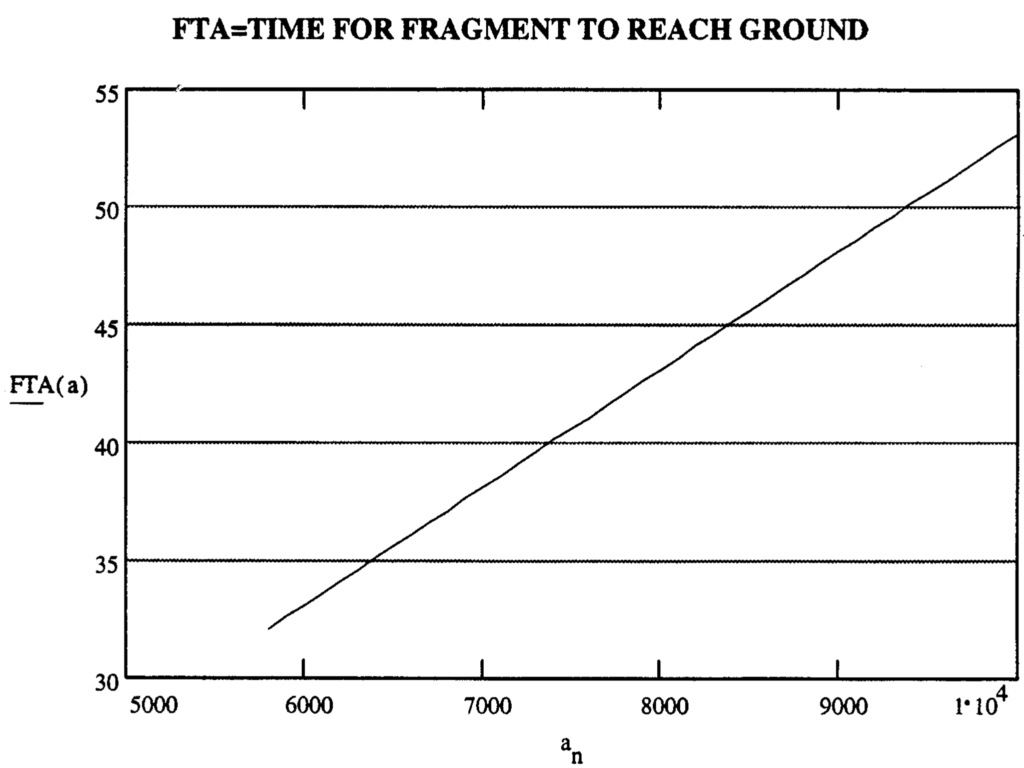

Figure C-25. GEMs Descent Time (Altitude > 5800 Feet).

FBG=MASS OF PROPELLANT BURNED ON THE GROUND

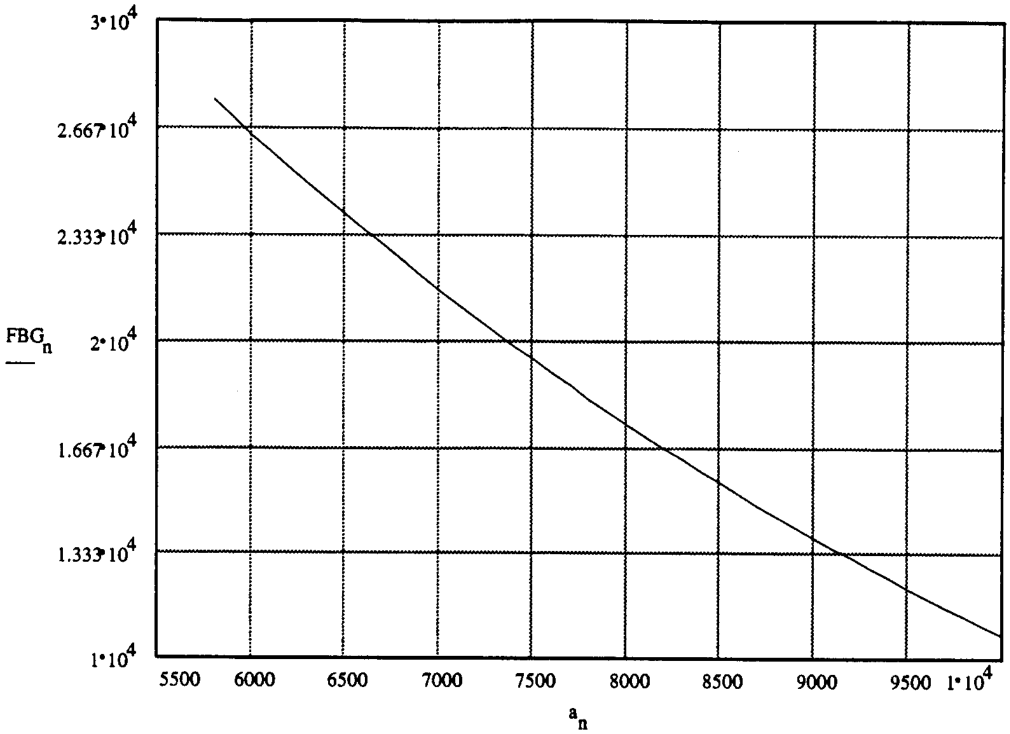

Figure C-26. Mass of GEMs Propellant Burned on the Ground (Altitude > 5800 Feet).

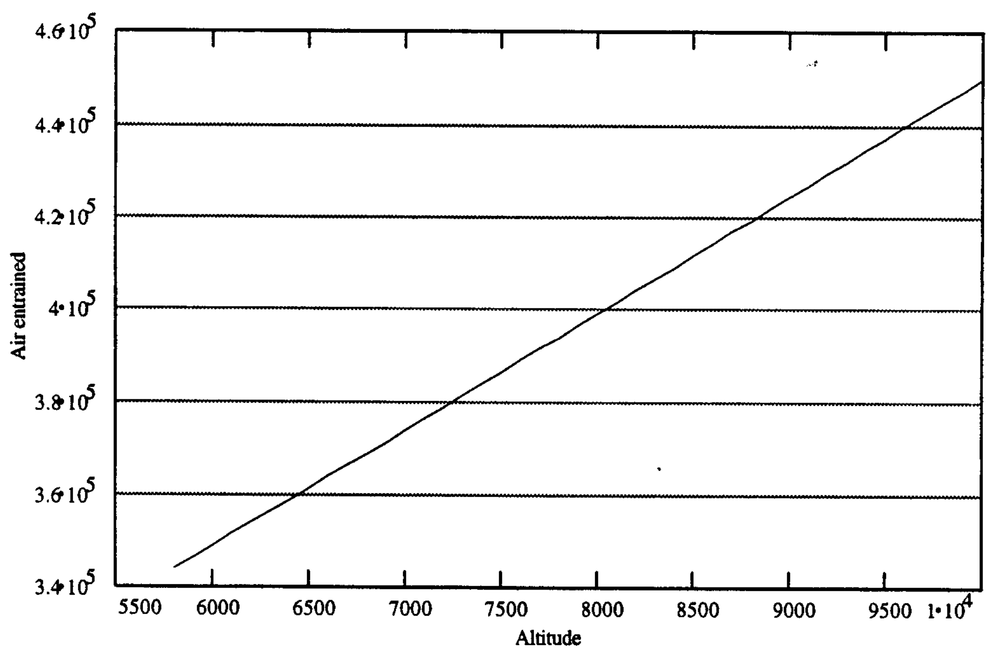

Figure C-27. GEMs Air Entrainment as a Function of Elevation (Altitude > 5800 Feet).

APPENDIX D

TITAN IV SOLID ROCKET PROPELLANT AIR ENTRAINMENT

The Titan IV air entrainment analysis is based upon the Delta II data presented in Appendix C, and scaled for the larger United Technologies Chemical Systems Division (CSD) solid rocket motors. This analysis is also based upon the Delta II RTI fragmentation data because no SRM fragmentation data or models are currently available for the Titan IV motors. Existing fragmentation data for the Titan IV CSD motors involves case fragmentation, not propellant fragmentation.

The following assumptions were used for this model.

A. Both SRMs are fragmented by either the exploding core vehicle or the destruct package.

B. The propellant fragments are cubic in shape and burn on all six sides.

C. All burning fragments are the mean size based upon initial burning surface area.

D. Average fragment initial vertical velocity is zero. Accounting for the forward velocity of the vehicle prior to abort was not considered in the model.

E. Fragments burning while descending in the air will entrain 100 percent by volume instantaneously due to the high turbulence.

F. Fragments burning on the ground will entrain 50 percent by volume prior to burnout.

G. Fragment terminal velocity is 200 feet per second.

H. The burn rate of the propellant at one atmosphere pressure is 0.11 inches per second. This is derived from the burn rate equation for the propellant at elevated pressures and applied at one atmosphere.

I. Based on these assumptions, the following steps were taken to develop the model.

1. The RTI data were scaled for the number, surface area, and size of the propellant fragments as a function of abort time in seconds for the Titan IV CSD solids.

2. A series of equations was developed which defined the pounds of propellant burned in the air and on the ground as a function of the time and elevation of the abort.

3. The model was segregated into two distinct phases.

a. 0-615 feet. For aborts in this elevation range, the fragments continually accelerate until they impact the ground.

b. 616-10,000 feet. The fragments reach terminal velocity before impacting the ground, and the motor fragments impact the ground and continue to burn there.

The following pages present the mathematical model generated.

TITAN IV CSD SOLIDS FRAGMENTATION AND BURNING FOR ABORTS BELOW 615 FEET ALTITUDE

$FSEU := .10$	**FRACTION SOLIDS ENTRAINED INTO UPPER CLOUD**	(D-1)
$n := 0..62$		
$a_n := 10 \cdot n$	**ELEVATION OF ABORT, FT.**	(D-2)
$s_n := \frac{6.5}{62} \cdot n$	**TIME OF ABORT, SEC. AFTER IGNITION**	(D-3)
$MSI := 592000 \cdot 2 \quad MSI = 1.184 \cdot 10^6$	**TOTALMASS OF SOLID PROPELLANT INITIAL, Lb.**	(D-4)
$BSDA := 5382 \cdot 2 \quad BSDA = 1.076 \cdot 10^4$	**TOTALBURN RATE OF SOLID DURING ASCENT, Lb./Sec**	(D-5)
$FNA(s) := -0.13 \cdot \left(s_n\right)^2 - 3.84 \cdot s_n + 1164.1$	**NUMBER OF FRAGMENTS PER SRM**	(D-6)
$FWA(s) := \frac{MSI - BSDA \cdot s_n}{FNA(s) \cdot 2}$	**FRAGMENT WEIGHT AT ABORT (LB)**	(D-7)
$FLA(s) := \left(\frac{FWA(s)}{0.06366}\right)^{\frac{1}{3}}$	**FRAGMENT CUBE EDGE DIMENSION (IN.)**	(D-8)
$FTA(a) := \sqrt{\frac{2 \cdot a_n}{32}}$	**FRAGMENT TIME FALLING THROUGH AIR**	(D-9)
$FBA_n := \left[\left[FLA(s)^3 - (FLA(s) - 0.22 \cdot FTA(a))^3\right] \cdot 0.06366\right] \cdot 2 \cdot FNA(s)$	**LB. FRAGMENTS BURNED WHILE FALLING**	(D-10)
$FBG_n := \left[\left(MSI - BSDA \cdot s_n\right) - FBA_n\right]$	**TOTAL MASS OF PROPELLANT BURNING ON THE GROUND**	(D-11)
$WPT_n := FBA_n + FBG_n + \left(BSDA \cdot s_n\right)$	**CHECK THAT TOTAL MASS OF PROPELLANT IS ACCOUNTED FOR AT ALL TIMES**	(D-12)
$AE(a) := \left(FBA_n + 0.5 \cdot FBG_n\right) \cdot (1 - FSEU)$	**AIR ENTRAINED INTO SOLIDS CLOUD**	(D-13)

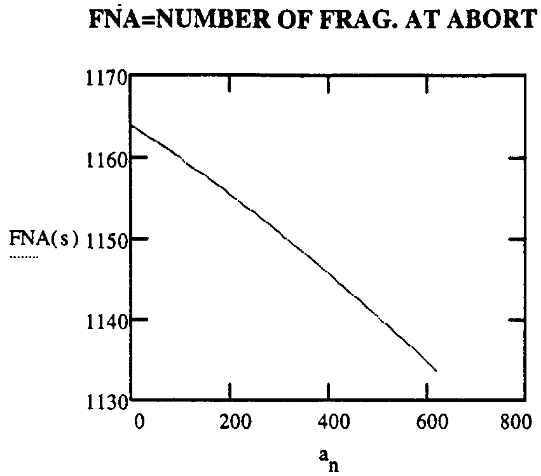

Figure D-1. Number of CSD Fragments (Altitude < 615 Feet).

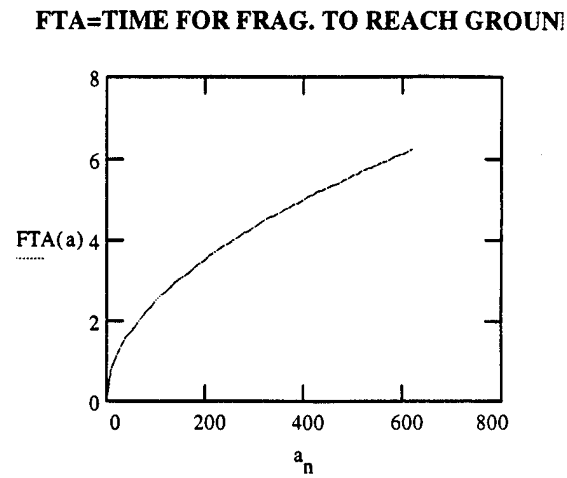

Figure D-2. CSD Descent Time (Altitude < 615 Feet).

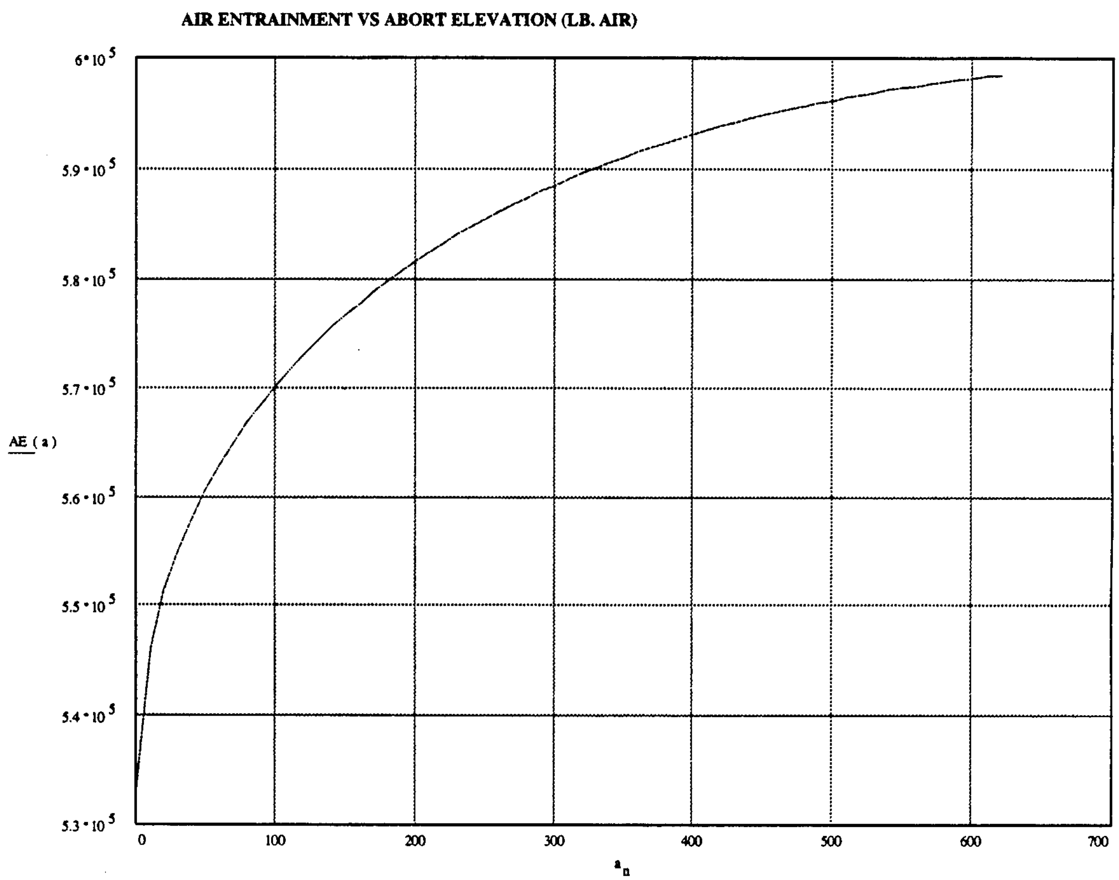

Figure D-3 CSD Air Entrainment (Altitude < 615 Feet).

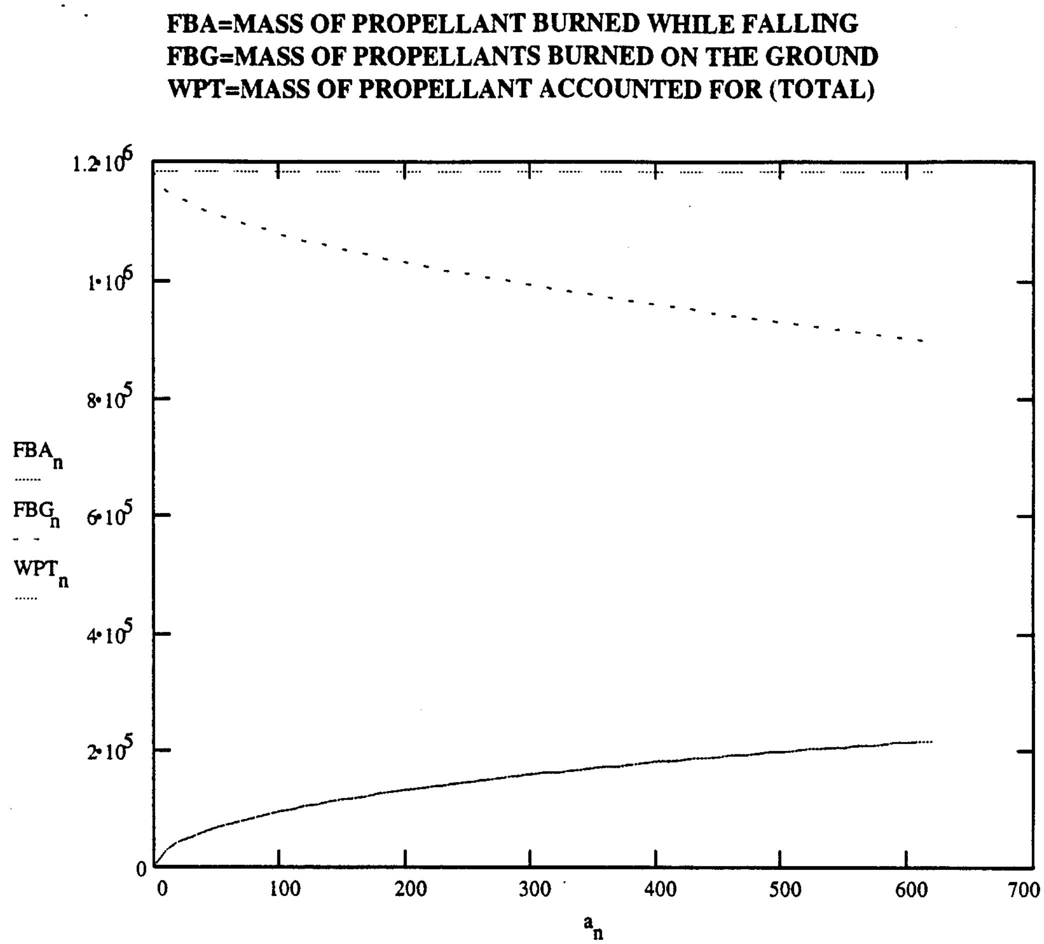

Figure D-4. Total Mass of CSD Propellant Burned (Altitude < 615 Feet).

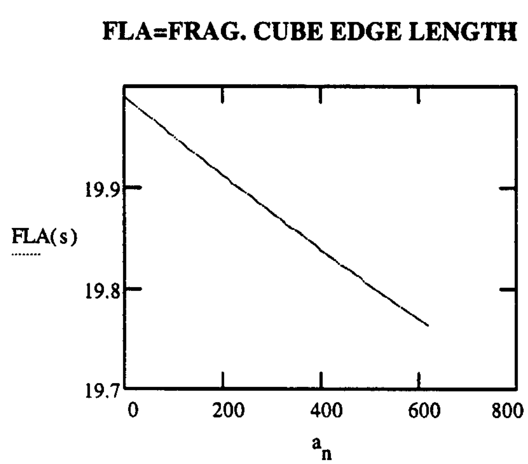

Figure D-5. CSD Fragment Cube Edge Length (Altitude < 615 Feet).

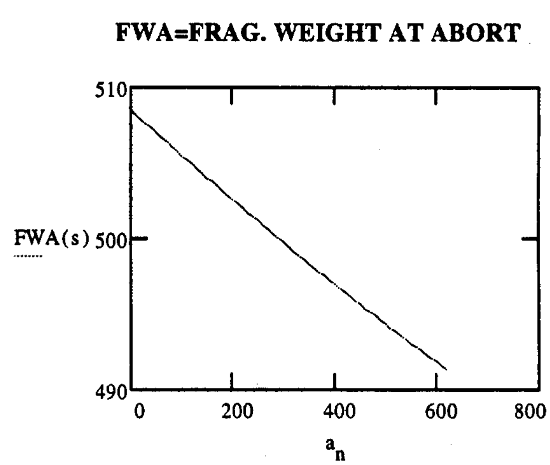

Figure D-6. CSD Fragment Weight (Altitude < 615 Feet).

TITAN IV CSD FRAGMENTATION AND BURNING FOR ABORTS FROM 615 TO 10,000 FEET ALTITUDE

$FSEU := .05$ $n := 1..94$	**FRACTION SOLIDS ENTRAINED INTO THE UPPER CLOUD**	(D-14)
$a_n := 615 + 100 \cdot n$	**ELEVATION OF ABORT, FT.**	(D-15)
$s_n := 6.5 + \left(\frac{35}{94}\right) \cdot n$	**TIME OF ABORT, SEC. AFTER IGNITION**	(D-16)
$MSI := 592000 \cdot 2$	**TOTALMASS OF SOLID PROPELLANT INITIAL, Lb.**	(D-17)
$BSDA := 5382 \cdot 2$	**TOTALBURN RATE OF SOLID DURING ASCENT, Lb./Sec.**	(D-18)
$FNA(s) := -0.13 \cdot (s_n)^2 - 3.84 \cdot s_n + 1164.1$	**NUMBER OF FRAGMENTS PER SRM**	(D-19)
$FWA(s) := \frac{MSI - BSDA \cdot s_n}{FNA(s) \cdot 2}$	**FRAGMENT WEIGHT AT ABORT (LB)**	(D-20)
$FLA(s) := \left(\frac{FWA(s)}{0.06366}\right)^{\frac{1}{3}}$	**FRAGMENT CUBE EDGE DIMENSION (IN.)**	(D-21)
$FTA(a) := 6.5 + \frac{a_n - 615}{200}$	**FRAGMENT TIME FALLING THROUGH AIR**	(D-22)
$FBA_n := \left[\left[FLA(s)^3 - (FLA(s) - 0.22 \cdot FTA(a))^3\right] \cdot 0.06366\right] \cdot 2 \cdot FNA(s)$	**LB. FRAGMENTS BURNED WHILE FALLING**	(D-23)
$FLAGI(a) := FLA(s) - 0.2 \cdot FTA(a)$	**FRAGMENT CUBE EDGE LENGTH AT GROUND IMPA(**	(D-24)
$FBG_n := \left[(MSI - BSDA \cdot s_n) - FBA_n\right]$	**TOTAL MASS OF PROPELLANT BURNING ON THE GROUND**	(D-25)
$WPT_n := FBA_n + FBG_n + (BSDA \cdot s_n)$	**CHECK THAT TOTAL MASS OF PROPELLANT IS ACCOUNTED FOR AT ALL TIMES**	(D-26)
$AE(a) := \left[(FBA_n) + 0.5 \cdot FBG_n\right] \cdot (1 - FSEU)$	**AIR ENTRAINED INTO SOLIDS CLOUD**	(D-27)

FLAGI= FRAGMENT CUBE EDGE LENGTH AT GROUND IMPACT, in.

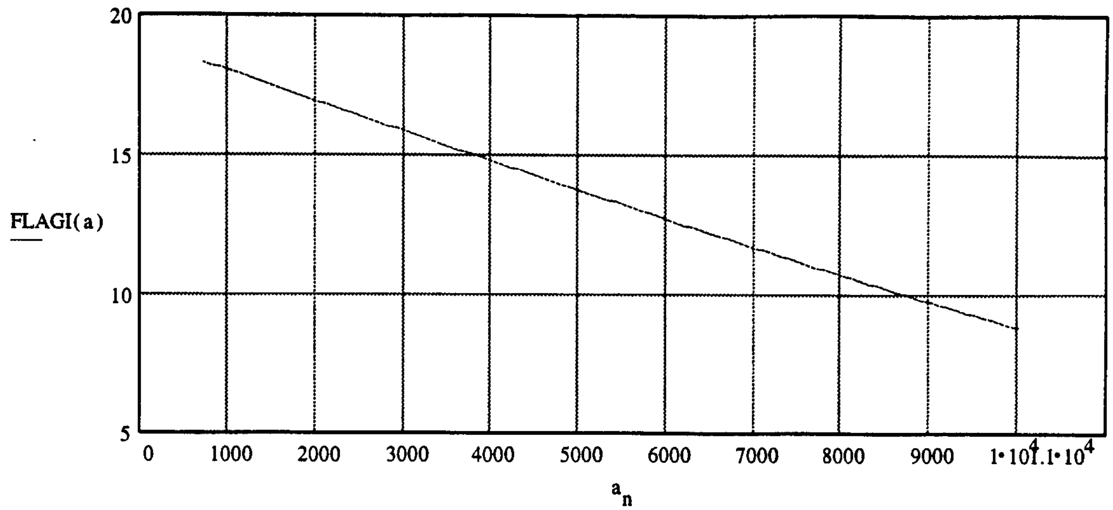

Figure D-7. CSD Fragment Cube Edge Length (615 - 10,000 Feet Altitude).

AE= AIR ENTRAINED INTO SOLIDS CLOUD, Lb.

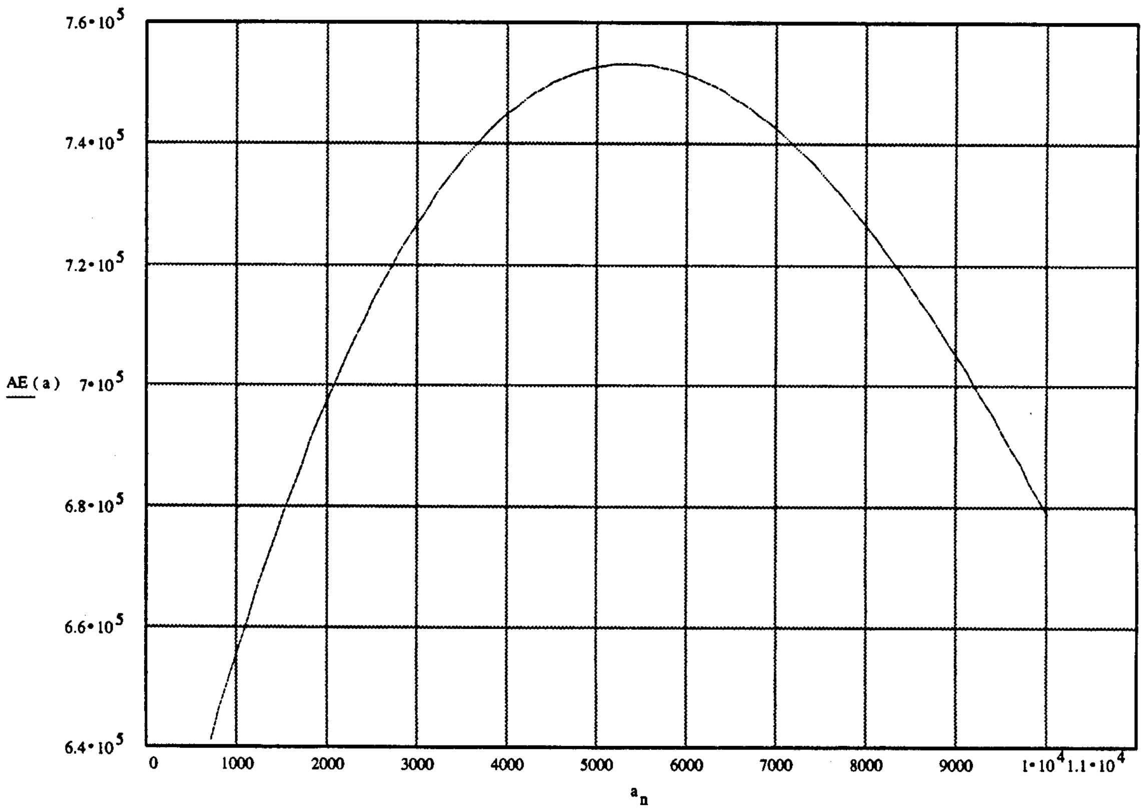

Figure D-8. CSD Air Entrainment as a Function of Elevation (615 - 10,000 Feet Altitude).

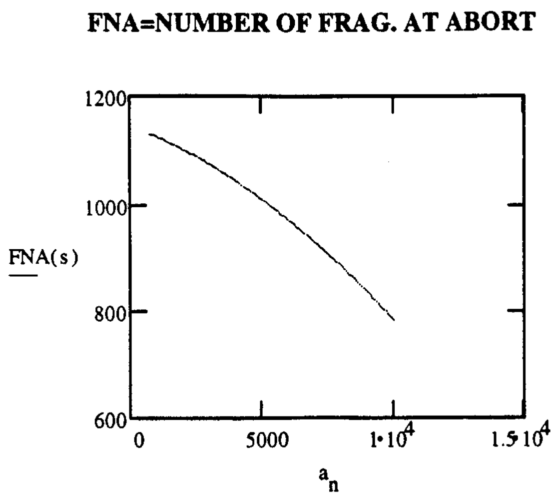

Figure D-9. Number of CSD Fragments (615 - 10,000 Feet Altitude).

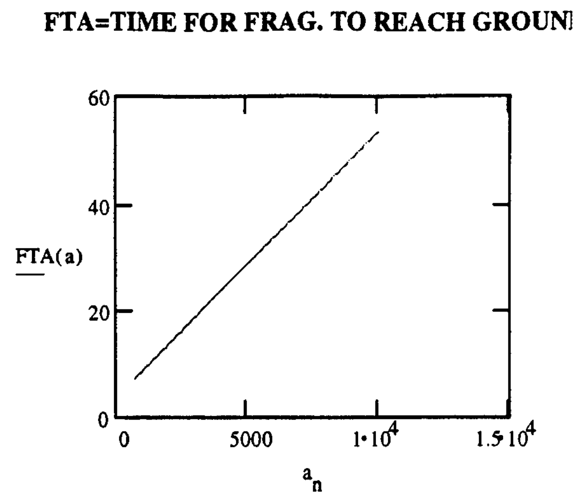

Figure D-10. CSD Descent Time (615 - 10,000 Feet Altitude).

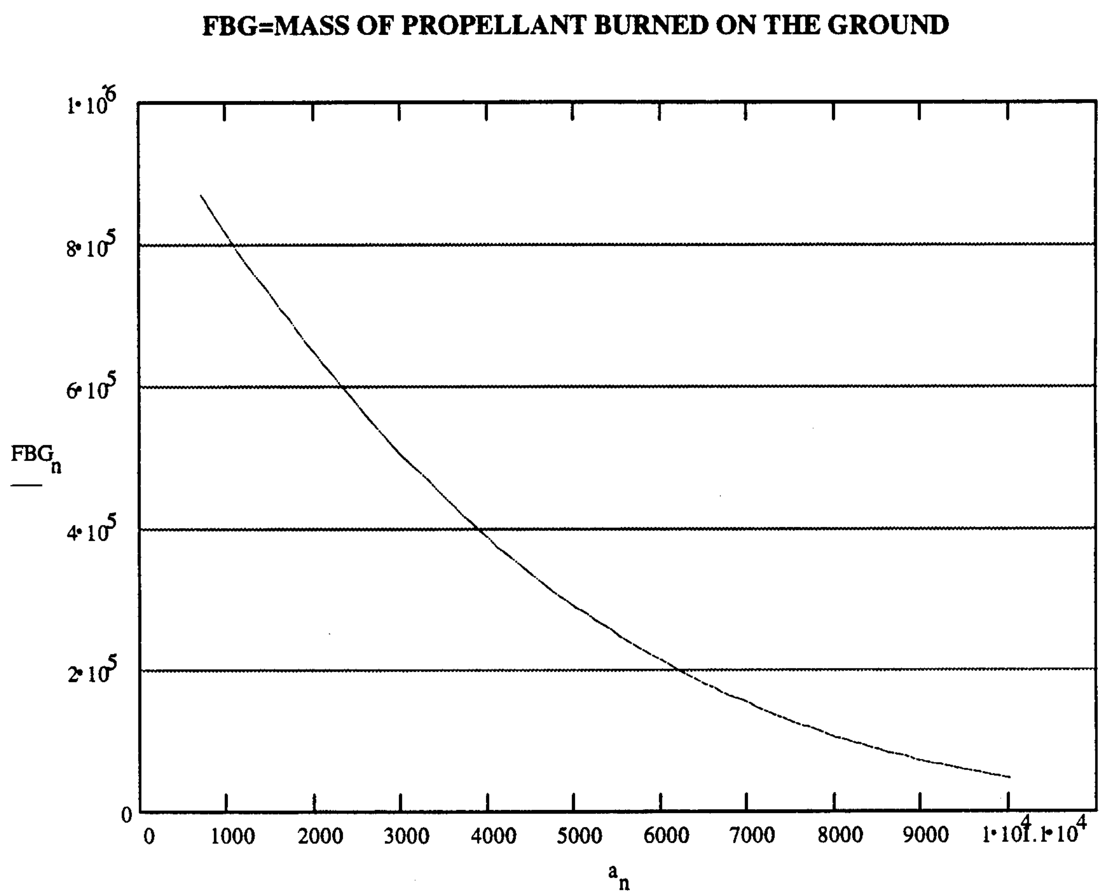

Figure D-11. Mass of CSD Propellant Burned on the Ground (615 - 10,000 Feet Altitude).

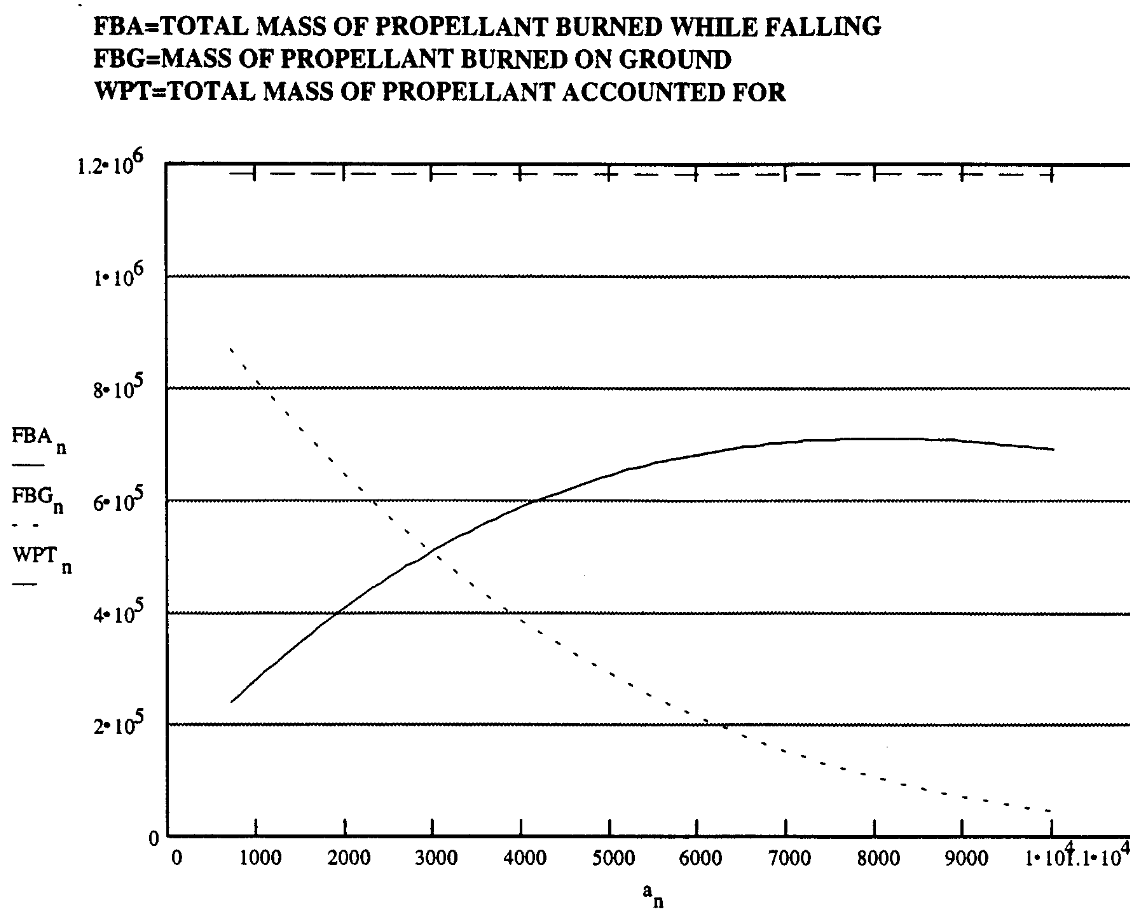

Figure D-12. Total Mass CSD Propellant Burned (615 - 10,000 Feet Altitude).

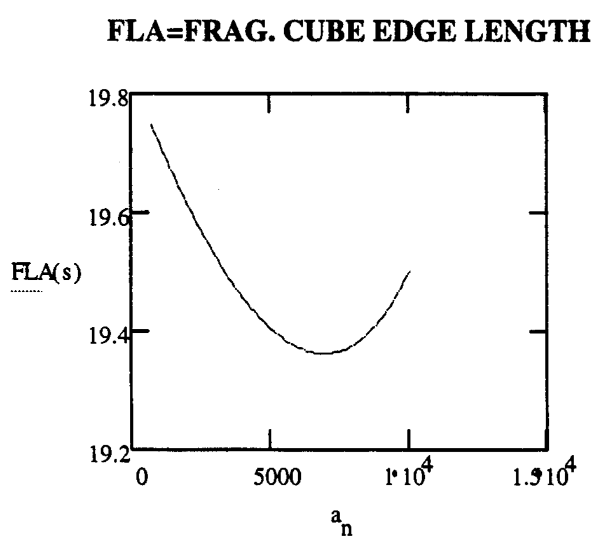

Figure D-13. CSD Fragment Cube Edge Length (615 - 10,000 Feet Altitude).

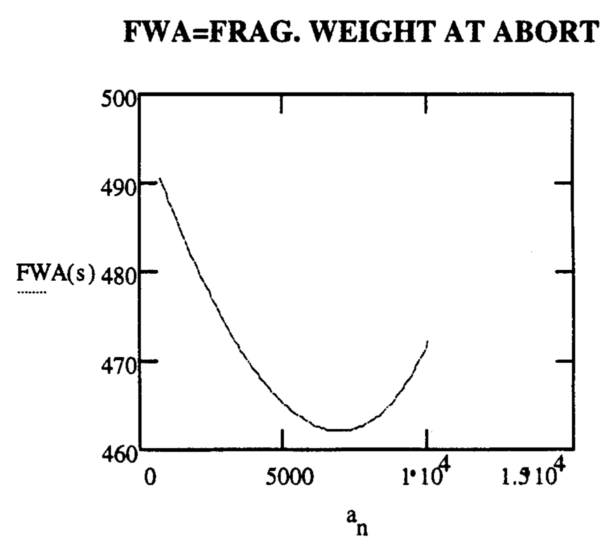

Figure D-14. CSD Fragment Weight (615 - 10,000 Feet Altitude).

APPENDIX E

FIREBALL ANALYSIS FOR DECOMPOSITION REACTIONS

To determine the extent of propellant thermal decomposition in an actively burning fireball, an estimate of the temperature profile is required. The percent of propellants above their respective auto-decomposition or monodecomposition temperatures can be determined.

The assumptions used for this analysis were:

A. The fireball is roughly spherical in shape.

B. The fireball size at burnout is based on the empirical correlations developed from Project Pyro.

C. The burning primarily occurs towards the center of the fireball, and the external surface of the fireball approaches but does not attain ambient temperature. The center of the fireball is at the adiabatic flame temperature expected for stoichiometric propellant combustion.

D. The temperature profile is linear with respect to fireball radius.

E. The chemical makeup of the fireball is homogeneous with respect to fireball radius. This assumption is necessary for the model development, although it is unrealistic.

F. The temperature and pressure gradients balance each other so that the profile of the fireball is constant.

G. The following thermal analysis was performed for the Delta II fireball.

1. For a nominal Delta II abort, the liquid fireball has the following characteristics.

   a. Fireball diameter = 496 feet; radius = 248 feet

   b. Average fireball temperature = 1594°C

   c. LOX/RP-1 stoichiometric flame temperature = 2790°C

2. Based upon the above assumptions and data, the following temperature profile is generated.

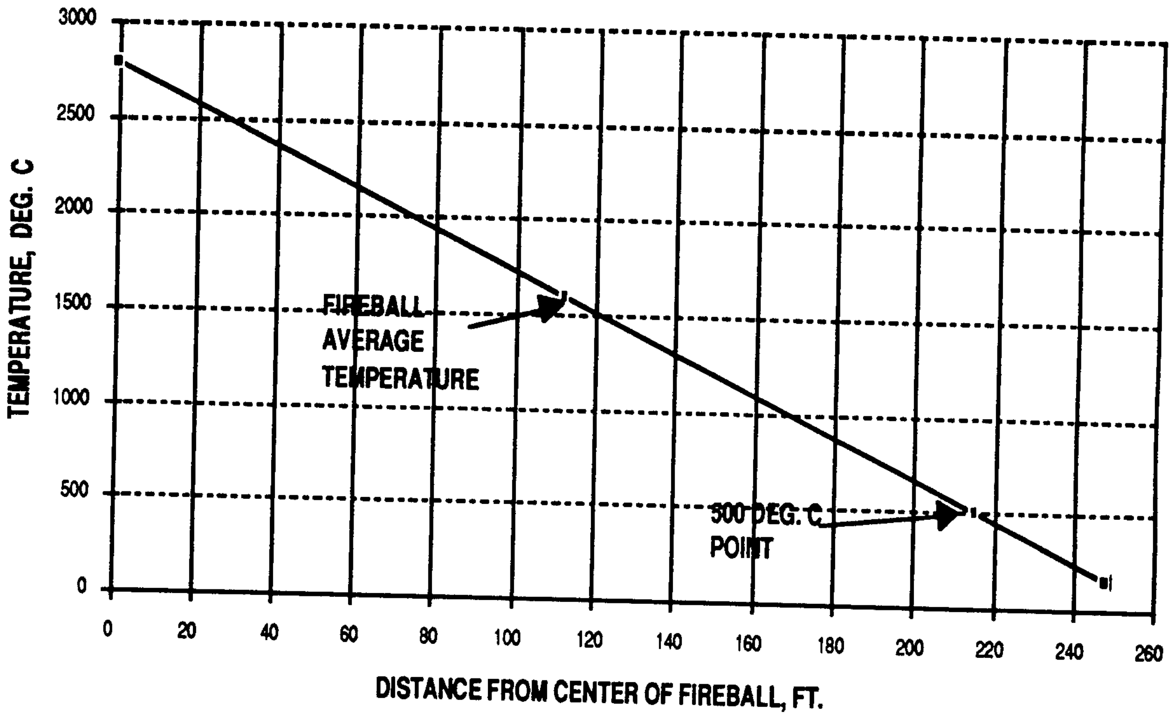

Figure E-1. Temperature vs. Fireball Radius, Delta II.

The temperature at which RP-1 undergoes thermal decomposition is 500°C. The temperature profile crosses the 500°C point at a radius of 219 feet. This implies that all RP-1 in the fireball inside the 215 foot radius is sufficiently hot to thermally decompose.

The total volume of the fireball = 4/3 * $(248)^3 = 6.39 \times 10^7$ ft^3.

The volume of the fireball above 500°C = 4/3 * $(219)^3 = 4.40 \times 10^7$ ft^3.

This implies that 69 percent of the fireball volume is above 500°C. The approximate amount of RP-1 that can be expected to thermally decompose in the fireball is therefore 70 percent.

H. The following thermal analysis was performed for the Titan IV fireball.

1. For a nominal Titan IV abort, the liquid fireball has the following characteristics.

a. Fireball diameter = 520 feet; radius = 260 feet

b. Average fireball temperature = 1025°C

c. A-50/N_2O_4 stoichiometric flame temperature = 2700°C

2. Based upon the above assumptions and data, the following temperature profile is generated.

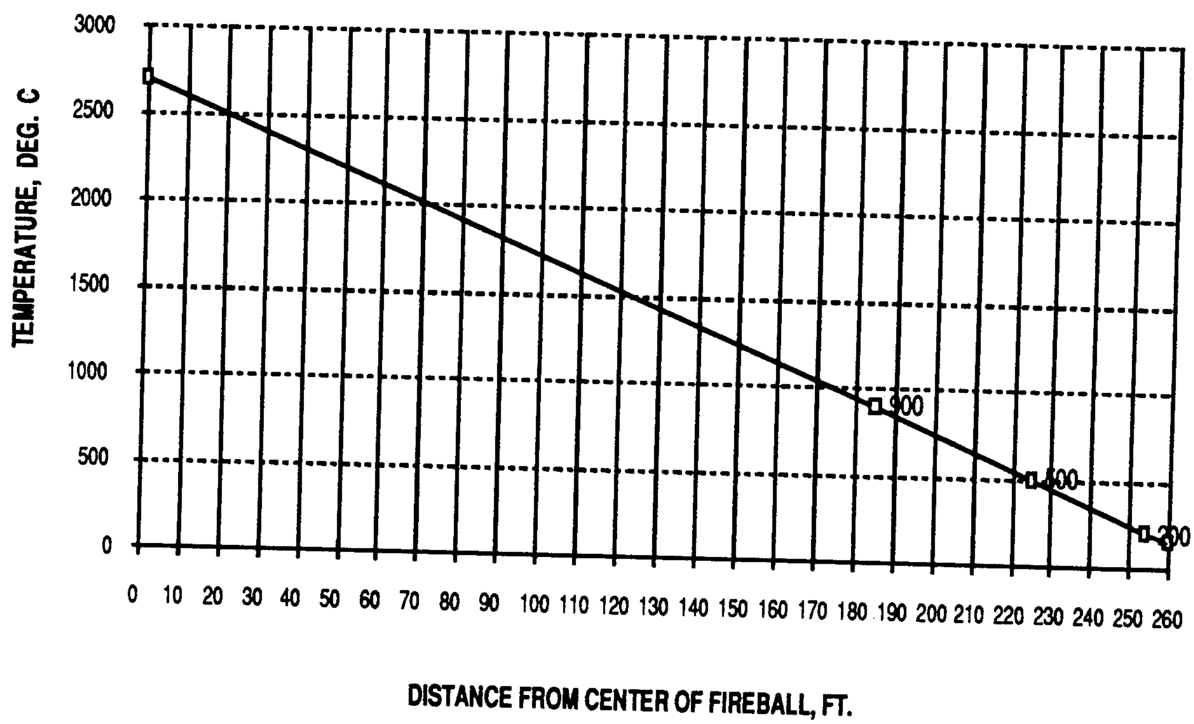

Figure E-2. Temperature vs. Fireball Radius, Titan IV.

UDMH thermally decomposes at 500°C, and Hydrazine monodecomposes at 200° C. The fireball cools to 500°C at a radius of 225 feet, and cools to 200°C at a radius of 255 feet.

The total volume of the fireball = $4/3 * (260)^3 = 7.36 \times 10^7$ ft^3.

The volume of the fireball above 500°C = $4/3 * (225)^3 = 4.77 \times 10^7$ ft^3.

The volume of the fireball above 200°C = $4/3 * (255)^3 = 6.95 \times 10^7$ ft^3.

This implies that 65 percent of the fireball exceeds 500°C, and 94 percent of the fireball exceeds 200°C. 65 percent of the UDMH and 94 percent of the hydrazine are expected to thermally decompose in the fireball.

APPENDIX F

THERMOCHEMICAL SPREADSHEETS FOR SOURCE MODELS

TABLE F-1. TITAN II COEFFICIENTS, CASE 1.

TITAN II SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
test case #1.		
on-pad abort, confined by ground surface, no air entrainment		
Variable	Description	Value
s	Time of Abort (from launch), seconds	0
A	Altitude at Abort, feet	0
γ	Liquid Propellant Reactivity Ratio	0.23
γ^*	Liquid Propellant Consumption Ratio	1
ζ	Air Entrainment Ratio, Liquids	0
ε	Fraction Excess Hydrazine Monodecomposed	0.94
η	Fraction Excess Hydrazine Vaporized	0.06
ξ	Fraction Excess UDMH Thermally Decomposed	0.65
ι	Fraction Excess UDMH Vaporized	0.35
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.35
SF	Scaling Factor	1.00143E+06

TABLE F-1. TITAN II COEFFICIENTS, CASE 1 (CONTINUED).

TITAN II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
test case #1.				
on-pad abort, confined by ground surface, no air entrainment				
Reactant Composition				
coefficient	value		comments	
a1	0.234991			
a2	0.275348			
a3	0.511361			
a4	0.079994			
a5	0		a5 must be less than or equal to	0.314206
a6	0.204234			
a7	0.109972			
a8	0.150006			
a9	0		a9 must be less than or equal to	0.589194
a10	0.553842			
a11	0.035352			
a12	0			
a13	0			

TABLE F-1. TITAN II COEFFICIENTS, CASE 1 (CONTINUED).

TITAN II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
test case #1.				
on-pad abort, confined by ground surface, no air entrainment				
Product Composition				
coefficient	value		comment	
b1	0.072424			
b2	0			
b3	0.087581			
b4	0.620118			
b5	0			
b6	0			
b7	0.276921			
b8	0.45593			
b9	0.276921			
b10	0			
b11	0.204234			
b12	0			
b13	0.275348			
b14	0			
b15	0.017507			
b16	0.034215			
b17	0			
b18	0.550696			
b19	0.553842			
b20	0.035352			
b21	0.408468			
b22	0.109972			
b23	0			
b24	1.022722			

TABLE F-1. TITAN II COEFFICIENTS, CASE 1 (CONCLUDED).

TITAN II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
test case #1.				
on-pad abort, confined by ground surface, no air entrainment				
SUMMARY				
REACTANTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt**
N2O4	1.0217	47.40847	207560	92.016
UDMH	0.3942	18.29149	52307	60.102
N2H4	0.7392	34.30003	52297	32.045
O2	0	0	0	31.999
N2	0	0	0	28.013
Total	2.1551	100	312165	
PRODUCTS				
CO2	0.072424	1.447833	7037	44.01
CO	0.087581	1.750835	5416	28.01
H2O	0.620118	12.39678	24664	18.015
H2	0.276921	5.535932	1233	2.016
N2	1.212433	24.23775	74985	28.013
NO	0.017507	0.349979	1160	30.006
O2	0.584911	11.69296	41322	31.999
NH3	0.553842	11.07186	20824	17.03
N2H4(g)	0.035352	0.706715	2501	32.045
CH4	0.408468	8.165681	14468	16.043
UDMH(g)	0.109972	2.198453	14592	60.102
N2O4(g)	0	0	0	92.016
NO2	1.022722	20.44523	103879	46.006
Total	5.00225	100	312081	
Adiabatic Flame Temperature,K				1342
Average Molecular Weight				28.26
Fireball Diameter, empirical, feet				562
Fireball Volume, empirical, cubic feet				9.2848E+07
Heat Released, calories				-5.5872E+10

TABLE F-2. TITAN II THERMAL PROPERTIES, CASE 1.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED:TITAN II MODEL-Test Case #1

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.7392	N2H4(l)	12054						
0.3942	UDMH(l)	12339						
1.0217	N2O4(l)	-4676						
0	C12 H26(l)	-84180						
0	O2(g)	0						
0	N2(g)	0						
0.0724	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.0876	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.6201	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0.2769	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
1.2124	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0	H	52094	1000-5000	4.9680E+00	0.0000E+00	0.0000E+00	0.0000E+00	-1.4800E+03
0	OH	9625	1000-5000	5.7850E+00	1.9060E-03	-3.8600E-07	2.7300E-11	-1.8050E+03
0	AlCl	-12300	1000-5000	8.6568E+00	4.2687E-04	-1.2602E-07	1.5323E-11	-2.5976E+03
0	Cl	28989	1000-5000	5.8811E+00	-8.3263E-04	3.1757E-07	-5.5844E-11	-1.7183E+03
0.5849	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0.0175	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0	O	59589	1000-5000	5.0520E+00	-5.5000E-05	-6.0000E-09	9.0000E-12	-1.5040E+03
0.5538	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0.11	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0.0354	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
1.0227	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0.4085	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03

TABLE F-2. TITAN II THERMAL PROPERTIES, CASE 1 (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN II MODEL - Case#1

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K) A	B	C	D	E
N2H4(l)	8910.3168						
UDMH(l)	4864.0338						
N2O4(l)	-4777.4692						
C12 H26(l)	0						
O2(g)	0						
N2(g)	0						
CO2	-6809.3648	273-3700	4.6285E-01	7.3124E-04	-2.4652E-07	0.0000E+00	-1.6826E+02
CO	-2314.0416	273-3700	5.6765E-01	1.3718E-04	-2.0936E-08	0.0000E+00	-1.7502E+02
H2O	-35840.5398	273-3700	4.3221E+00	2.1480E-03	-3.0013E-07	0.0000E+00	-1.3810E+03
H2	0	273-3700	1.7788E+00	2.8770E-04	-2.1598E-08	0.0000E+00	-5.4272E+02
N2	0	273-3700	7.9158E+00	1.8041E-03	-2.7521E-07	0.0000E+00	-2.4369E+03
HCl	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Al2O3(S)	0	2315-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
H	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
OH	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
AlCl	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Cl	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
O2	0	273-3700	3.9375E+00	8.8027E-04	-1.0470E-07	0.0000E+00	-1.2113E+03
NO	378	273-3700	1.1309E-01	4.1265E-05	-1.3475E-08	1.5278E-12	-3.5420E+01
O	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NH3	-6113.952	273-1500	3.6473E+00	3.3926E-03	1.3103E-06	-8.8497E-10	-1.2477E+03
UDMH(g)	2277.55	0-2000	4.4660E-01	7.1940E-03	-2.3980E-06	0.0000E+00	-4.3131E+02
N2H4(g)	794.1636	273-330	3.5825E-01	6.5490E-04	-2.3647E-07	3.9613E-11	-1.3381E+02
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO2(g)	8140.692	273-1500	5.6054E+00	1.3970E-02	-8.6111E-06	1.9227E-09	-2.2193E+03
CH4	-7307.6565	1000-5000	1.2199E+00	8.4564E-03	-3.1757E-06	5.5021E-10	-7.1206E+02

TABLE F-2. TITAN II THERMAL PROPERTIES, CASE 1 (CONCLUDED).

A	B/2	C/3	D/4	E
3.0375E+01	1.9849E-02	-4.6979E-06	4.0726E-10	-1.0695E+04

HEAT OF FORMATION, REACTANTS (calories)	8996.8814
HEAT OF FORMATION, PRODUCTS (calories)	-46795.1491
HEAT OF REACTION, (calories)	-55792.0305
FLAME TEMPERATURE (K)	1342

TABLE F-3. TITAN II COEFFICIENTS, CASE 2.

TITAN II SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
test case #2.		
Abort at 5000 ft,20 sec,0.5 moles air/mole liquid propellants, command destruct		
Variable	Description	Value
s	Time of Abort (from launch), seconds	20
A	Altitude at Abort, feet	5000
γ	Liquid Propellant Reactivity Ratio	0.23
$\gamma*$	Liquid Propellant Consumption Ratio	0.89
ζ	Air Entrainment Ratio, Liquids	0.5
ε	Fraction Excess Hydrazine Monodecomposed	0.94
η	Fraction Excess Hydrazine Vaporized	0.06
ξ	Fraction Excess UDMH Thermally Decomposed	0.65
ι	Fraction Excess UDMH Vaporized	0.35
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.35
SF	Scaling Factor	1.00143E+06

TABLE F-3. TITAN II COEFFICIENTS, CASE 2 (CONTINUED).

TITAN II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
test case #2.				
Abort at 5000 ft,20 sec,0.5 moles air/mole liquid propellants, command destruct				
Reactant Composition				
coefficient	value		comments	
a1	0.209142			
a2	0.24506			
a3	0.455111			
a4	0.071195			
a5	0.020141		a5 must be less than or equal to	0.27964334
a6	0.168677			
a7	0.090826			
a8	0.133505			
a9	0.020141		a9 must be less than or equal to	0.52438266
a10	0.473987			
a11	0.030255			
a12	0.201407			
a13	0.757613			

TABLE F-3. TITAN II COEFFICIENTS, CASE 2 (CONTINUED).

TITAN II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
test case #2.				
Abort at 5000 ft,20 sec,0.5 moles air/mole liquid propellants, command destruct				
Product Composition				
coefficient	value		comment	
b1	0.064458			
b2	0.040281			
b3	0.077947			
b4	0.551905			
b5	0.040281			
b6	0.0805628			
b7	0.236994			
b8	0.405777			
b9	0.236994			
b10	0.020141			
b11	0.168677			
b12	0.020141			
b13	0.24506			
b14	0.757613			
b15	0.015581			
b16	0.030451			
b17	0.100704			
b18	0.49012			
b19	0.473987			
b20	0.030255			
b21	0.337353			
b22	0.090826			
b23	0			
b24	0.910222			

TABLE F-3. TITAN II COEFFICIENTS, CASE 2 (CONCLUDED).

TITAN II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
test case #2.				
Abort at 5000 ft,20 sec,0.5 moles air/mole liquid propellants, command destruct				
SUMMARY				
REACTANTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
N2O4	0.909313	31.60564	184728	92.016
UDMH	0.350838	12.19433	46554	60.102
N2H4	0.657888	22.86668	46545	32.045
O2	0.201407	7.000447	14229	31.999
N2	0.757613	26.33288	46856	28.013
Total	2.877059	99.99998	338911	
PRODUCTS				
CO2	0.104739	1.930199	10177	44.01
CO	0.077947	1.436463	4820	28.01
H2O	0.672749	12.39787	26757	18.015
H2	0.236994	4.367478	1055	2.016
N2	1.854401	34.17414	114689	28.013
NO	0.015581	0.287138	1032	30.006
O2	0.621274	11.44926	43891	31.999
NH3	0.473987	8.734956	17821	17.03
N2H4(g)	0.030255	0.55755	2140	32.045
CH4	0.337353	6.216973	11949	16.043
UDMH(g)	0.090826	1.673801	12052	60.102
N2O4(g)	0	0	0	92.016
NO2	0.910222	16.77418	92453	46.006
Total	5.426329	100	338837	
Adiabatic Flame Termperature, K				1384
Average Molecular Weight				28.28
Fireball Diameter, empirical, feet				541
Fireball Volume, empirical, cubic feet				8.2789E+07
Heat Released, calories				-6.001E+10

TABLE F-4. TITAN II THERMAL PROPERTIES, CASE 2.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED:TITAN II MODEL-Test Case #2

MOL COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.6579	N2H4(l)	12054						
0.3508	UDMH(l)	12339						
0.9093	N2O4(l)	-4676						
0	C12 H26(l)	-84180						
0.2014	O2(g)	0						
0.7576	N2(g)	0						
0.1047	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.0779	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.6727	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0.237	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
1.8544	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0	H	52094	1000-5000	4.9680E+00	0.0000E+00	0.0000E+00	0.0000E+00	-1.4800E+03
0	OH	9625	1000-5000	5.7850E+00	1.9060E-03	-3.8600E-07	2.7300E-11	-1.8050E+03
0	AlCl	-12300	1000-5000	8.6568E+00	4.2687E-04	-1.2602E-07	1.5323E-11	-2.5976E+03
0	Cl	28989	1000-5000	5.8811E+00	-8.3263E-04	3.1757E-07	-5.5844E-11	-1.7183E+03
0.6213	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0.0156	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0	O	59589	1000-5000	5.0520E+00	-5.5000E-05	-6.0000E-09	9.0000E-12	-1.5040E+03
0.474	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0.0908	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0.0303	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0.9102	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0.3374	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03

TABLE F-4. TITAN II THERMAL PROPERTIES, CASE 2 (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN II MODEL - Case#2

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K)				
			A	B	C	D	E
N2H4(l)	7930.3266						
UDMH(l)	4328.5212						
N2O4(l)	-4251.8868						
C12 H26(l)	0						
O2(g)	0						
N2(g)	0						
CO2	-9847.2444	273-3700	6.6935E-01	1.0575E-03	-3.5650E-07	0.0000E+00	-2.4332E+02
CO	-2057.8064	273-3700	5.0479E-01	1.2199E-04	-1.8618E-08	0.0000E+00	-1.5564E+02
H2O	-38880.7146	273-3700	4.6887E+00	2.3302E-03	-3.2559E-07	0.0000E+00	-1.4981E+03
H2	0	273-3700	1.5225E+00	2.4624E-04	-1.8486E-08	0.0000E+00	-4.6452E+02
N2	0	273-3700	1.2107E+01	2.7593E-03	-4.2095E-07	0.0000E+00	-3.7273E+03
HCl	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Al2O3(S)	0	2315-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
H	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
OH	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
AlCl	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Cl	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
O2	0	273-3700	4.1826E+00	9.3506E-04	-1.1121E-07	0.0000E+00	-1.2867E+03
NO	336.96	273-3700	1.0081E-01	3.6785E-05	-1.2012E-08	1.3619E-12	-3.1574E+01
O	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NH3	-5232.96	273-1500	3.1218E+00	2.9037E-03	1.1215E-06	-7.5745E-10	-1.0679E+03
UDMH(g)	1880.014	0-2000	3.6865E-01	5.9383E-03	-1.9794E-06	0.0000E+00	-3.5603E+02
N2H4(g)	679.7502	273-330	3.0664E-01	5.6055E-04	-2.0240E-07	3.3906E-11	-1.1453E+02
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO2(g)	7245.192	273-1500	4.9888E+00	1.2433E-02	-7.6639E-06	1.7112E-09	-1.9751E+03
CH4	-6035.7486	1000-5000	1.0075E+00	6.9845E-03	-2.6229E-06	4.5444E-10	-5.8812E+02

TABLE F-4. TITAN II THERMAL PROPERTIES, CASE 2 (CONCLUDED).

A	B/2	C/3	D/4	E
3.3570E+01	1.8154E-02	-4.2035E-06	3.6086E-10	-1.1509E+04

HEAT OF FORMATION, REACTANTS (calories)	8006.961
HEAT OF FORMATION, PRODUCTS (calories)	-51912.5578
HEAT OF REACTION, (calories)	-59919.5188
FLAME TEMPERATURE (K)	1384

TABLE F-5. DELTA II COEFFICIENTS, CASE 1, UPPER CLOUD.

DELTA II SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
UPPER CLOUD		
test case #1.		
On-pad abort, confined by ground surface, no air entrainment in liquid cloud		
Variable	Description	Value
s	Time of Abort (from launch), seconds	0
A	Altitude at Abort, feet	0
α	Fraction Total Liquids in Cloud	1
β	Fraction Total Solids in Cloud	0.1
δ	Solid Propellant Reactivity Ratio	1
$\delta*$	Solid Propellant Consumption Ratio	1
γl	Liquid Propellant Reactivity Ratio, LOX/RP-1	0.44
$\gamma l*$	Liquid Propellant Consumption Ratio, LOX/RP-1	1
γ	Liquid Propellant Reactivity Ratio, N2O4/A-50	0.229
$\gamma*$	Liquid Propellant Consumption Ration, N2O4/A-50	1
ζ	Air Entrainment Ratio, Liquids	0
ε	Fraction Excess Hydrazine Monodecomposed	0.94
η	Fraction Excess Hydrazine Vaporized	0.06
ξ	Fraction Excess UDMH Thermally Decomposed	0.7
ι	Fraction Excess UDMH Vaporized	0.3
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.35
μ	Fraction Excess RP-1 Thermall Decomposed (cracking)	0.75
υ	Fraction Excess RP-1 Vaporized	0.25
π	Fraction of Solids which Entrain Air	0
ρ	Air Entrainment Ratio, Solids	2.9248
σ	HCl Reactivity	1
SF	Scaling Factor	6.4702E+06

TABLE F-5. DELTA II COEFFICIENTS, CASE 1, UPPER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
UPPER CLOUD				
test case #1.				
On-pad abort, confined by ground surface, no air entrainment in liquid cloud				
Reactant Composition				
coefficient	value		comments	
a1	0.00965			
a2	0.01341			
a3	0.01156			
a4	0			
a5	0			
a6	0			
a7	0			
a8	0.140932			
a9	0		a9 must be less than or equal to	0.193668
a10	0.145251			
a11	0.048417			
a12	0.001534			
a13	0.004825			
a14	0.000119			
a15	0.000221			
a16	0.00052			
a17	0		a17 must be less than or equal to	0.00218571
a18	0.00153			
a19	0.000656			
a20	0.000976			
a21	0		a21 must be less than or equal to	0.00410006
a22	0.003854			
a23	0.000246			
a24	0.140932			
a25	0.179368			

TABLE F-5. DELTA II COEFFICIENTS, CASE 1, UPPER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
UPPER CLOUD				
test case #1.				
On-pad abort, confined by ground surface, no air entrainment in liquid cloud				
Product Composition				
coefficient	value		comment	
b1	0.048225			
b2	0			
b3	0			
b4	0.107051			
b5	0.105538			
b6	0			
b7	0			
b8	0			
b9	0			
b10	0.046973			
b11	0.017674		b11 must be > or = to 0	
b12	0.001927			
b13	0.007781			
b14	0.001927			
b15	0			
b16	0.00153			
b17	0			
b18	0.000119			
b19	0			
b20	0			
b21	0.00467			
b22	0.005538			
b23	0.000114			
b24	0.000223			
b25	0.179368			
b26	0			
b27	0			
b28	0.000238			
b29	0.003854			
b30	0.000246			
b31	0.00306			
b32	0.000656			
b33	0.072626			
b34	0.004035			
b35	0			
b36	0.000443			
b37	0.004825			
b38	0.004825			

TABLE F-5. DELTA II COEFFICIENTS, CASE 1, UPPER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
UPPER CLOUD				
test case #1				
On-pad abort, confined by ground surface, no air entrainment in liquid cloud				
SUMMARY				
Consumed	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
O2(l)	0	#DIV/0!	0	31.999
RP-1(l)	0	#DIV/0!	0	13.976
NH4ClO4(s)	0	#DIV/0!	0	117.489
CH1.622(s)	0	#DIV/0!	0	13.646
Al(s)	0	#DIV/0!	0	26.982
Total	0			
REACTANTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
NH4ClO4	0.00965	1.370735	16173	117.489
CH1.622	0.01341	1.904824	2610	13.646
Al	0.01156	1.642041	4449	26.982
O2(l)	0.3203	45.49703	146200	31.999
O2(g)	0	0	0	31.999
N2	0	0	0	28.013
RP-1	0.3346	47.52827	66706	13.976
N2O4	0.0067	0.951702	8794	92.016
UDMH	0.002706	0.384374	2320	60.102
N2H4	0.005076	0.720964	2320	32.045
Total	0.704002	99.99994	249572	
PRODUCTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
CO2	0.048225	7.735021	30275	44.01
CO	0.107051	17.17032	42772	28.01
H2O	0.105538	16.92765	27121	18.015
H2	0.066574	10.67799	1914	2.016
N2	0.011357	1.821573	4538	28.013
HCl	0.00467	0.749057	2429	36.461
Al2O3	0.005538	0.888282	8055	101.961
NO	0.000114	0.018334	49	30.006
O2	0.17983	28.84358	82083	31.999
NH3	0.003854	0.618166	936	17.03
N2H4(g)	0.000246	0.039457	112	32.045
CH4	0.00306	0.490804	700	16.043
UDMH(g)	0.000656	0.105172	562	60.102
C2H4	0.072626	11.64867	29063	28.054
C12H26(g)	0.004035	0.647122	9803	170.337
N2O4(g)	0	0	0	92.016
NO2	0.000443	0.07104	291	46.006
HNO3	0.004825	0.773899	4337	63.013
NOCl	0.004825	0.773899	4505	65.451
Total	0.623466	100	249544	

TABLE F-5. DELTA II COEFFICIENTS, CASE 1, UPPER CLOUD (CONCLUDED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
UPPER CLOUD				
test case #1.				
On-pad abort, confined by ground surface, no air entrainment in liquid cloud				
Adiabatic Flame Temperature, K				1882
Average Molecular Weight (all products), lbs/lb-mole				28.06
Average Molecular Weight (gas products only), lbs/lb-mole				27.40
Fireball Diameter, empirical, feet				522
Fireball Volume, empirical, cubic feet				7.4495E+07
Fireball Diameter, ideal gas, feet				347
Fireball Volume, ideal gas, cubic feet				2.1799E+07
Total Heat Release, calories				-7.4848E+10

TABLE F-6. DELTA II THERMAL PROPERTIES, CASE 1, UPPER CLOUD.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #1 (upper cloud)

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.00965	NH4ClO4(s)	-70690						
0.01341	CH1.622(s)	-4241						
0.01156	Al(s)	0						
0.3203	O2(l)	-3124						
0	O2(g)	0						
0.3346	CH1.95	-6220						
0.0067	N2O4(l)	-4676						
0.002706	UDMH(l)	12339						
0.005076	N2H4(l)	12054						
0	N2(g)	0						
0.048225	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.107051	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.105538	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0.066574	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
0.011357	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0.00467	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0.005538	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0.000114	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0.17983	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0.003854	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0.00306	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
0.072626	C2H4(g)	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
0.000443	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0.004825	HNO3(g)	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
0.004825	NOCl(g)	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
0.000246	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0.000656	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0.004035	C12H26(g)	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04

TABLE F-6. DELTA II THERMAL PROPERTIES, CASE 1, UPPER CLOUD (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #1 (upper cloud)

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K) A	B	C	D	E
NH4ClO4(s)	-682.1585						
CH1.622(s)	-56.87181						
Al(s)	0						
O2(l)	-1000.6172						
O2(g)	0						
CH1.95	-2081.212						
N2O4(l)	-31.3292						
UDMH(l)	33.389334						
N2H4(l)	61.186104						
N2(g)	0						
CO2	-4535.6577	273-3700	3.0830E-01	4.8707E-04	-1.6421E-07	0.0000E+00	-1.1207E+02
CO	-2827.859216	273-3700	6.9369E-01	1.6764E-04	-2.5585E-08	0.0000E+00	-2.1389E+02
H2O	-6099.885324	273-3700	7.3560E-01	3.6558E-04	-5.1080E-08	0.0000E+00	-2.3503E+02
H2	0	273-3700	4.2767E-01	6.9170E-05	-5.1928E-09	0.0000E+00	-1.3049E+02
N2	0	273-3700	7.4150E-02	1.6899E-05	-2.5780E-09	0.0000E+00	-2.2828E+01
HCl	-103.02954	1000-5000	2.5676E-02	1.3347E-05	-4.3618E-09	6.8229E-13	-8.2052E+00
Al2O3(s)	-2217.969	1000-2315	1.3800E-01	2.9141E-05	-1.2383E-11	-2.7953E-12	-4.2432E+01
NO	2.4624	273-3700	7.3667E-04	2.6881E-07	-8.7780E-11	9.9522E-15	-2.3074E-01
O2	0	273-3700	1.2106E+00	2.7064E-04	-3.2190E-08	0.0000E+00	-3.7243E+02
NH3	-42.54816	273-1500	2.5382E-02	2.3610E-05	9.1186E-09	-6.1587E-12	-8.6831E+00
CH4	-54.74034	1000-5000	9.1378E-03	6.3345E-05	-2.3788E-08	4.1215E-12	-5.3339E+00
C2H4(g)	907.534496	1000-5000	4.9866E-01	1.6586E-03	-6.2996E-07	1.0991E-10	-2.1690E+02
NO2(g)	3.52628	273-1500	2.4281E-03	6.0514E-06	-3.7301E-09	8.3284E-13	-9.6131E-01
HNO3(g)	-155.751	0-1000	4.6306E-02	6.6199E-05	-2.4361E-08	0.0000E+00	-1.6521E+01
NOCl(g)	59.637	1000-5000	5.1965E-02	1.7389E-05	-6.4124E-09	1.1792E-12	-1.6202E+01
N2H4(g)	5.518764	1000-5000	2.4895E-03	4.5510E-06	-1.6433E-09	2.7527E-13	-9.2988E-01
UDMH(g)	13.58248	0-2000	2.6634E-03	4.2902E-05	-1.4301E-08	0.0000E+00	-2.5722E+00
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C12H26(g)	-280.53741	>270	2.0830E-02	1.0350E-03	-5.5175E-07	1.1391E-10	-4.7520E+01

TABLE F-6. DELTA II THERMAL PROPERTIES, CASE 1, UPPER CLOUD (CONCLUDED).

FIREBALL THERMAL PROPERTIES
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #1 (upper cloud)

A	B/2	C/3	D/4	E
4.2743E+00	2.1687E-03	-5.1071E-07	5.5492E-11	-1.4532E+03

HEAT OF FORMATION, REACTANTS (calories)	-3757.61327
HEAT OF FORMATION, PRODUCTS (calories)	-15325.7163
HEAT OF REACTION, (calories)	-11568.103
FLAME TEMPERATURE (K)	1882

ΔHr+AT+B/2T^2+C/3T^3+D/4T^4+E
-3.977424642

TABLE F-7. DELTA II COEFFICIENTS, CASE 1, LOWER CLOUD.

DELTA II SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
LOWER CLOUD		
test case #1.		
On-pad abort, confined by ground surface, no air entrainment in liquid cloud		
Variable	Description	Value
s	Time of Abort (from launch), seconds	0
A	Altitude at Abort, feet	0
α	Fraction Total Liquids in Cloud	0
β	Fraction Total Solids in Cloud	0.9
δ	Solid Propellant Reactivity Ratio	1
δ*	Solid Propellant Consumption Ratio	1
γl	Liquid Propellant Reactivity Ratio, LOX/RP-1	0.44
γl*	Liquid Propellant Consumption Ratio, LOX/RP-1	1
γ	Liquid Propellant Reactivity Ratio, N2O4/A-50	0.229
γ*	Liquid Propellant Consumption Ration, N2O4/A-50	1
ζ	Air Entrainment Ratio, Liquids	0
ε	Fraction Excess Hydrazine Monodecomposed	0.94
η	Fraction Excess Hydrazine Vaporized	0.06
ξ	Fraction Excess UDMH Thermally Decomposed	0.7
ι	Fraction Excess UDMH Vaporized	0.3
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.35
μ	Fraction Excess RP-1 Thermall Decomposed (cracking)	0.75
υ	Fraction Excess RP-1 Vaporized	0.25
π	Fraction of Solids which Entrain Air	1
ρ	Air Entrainment Ratio, Solids	2.92484308
σ	HCl Reactivity	0
SF	Scaling Factor	6.4656E+06

TABLE F-7. DELTA II COEFFICIENTS, CASE 1, LOWER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
LOWER CLOUD				
test case #1.				
On-pad abort, confined by ground surface, no air entrainment in liquid cloud				
Reactant Composition				
coefficient	value		comments	
a1	0.08685			
a2	0.12069			
a3	0.10404			
a4	0			
a5	0.053345			
a6	0			
a7	0.200678			
a8	0			
a9	0		a9 must be less than or equal to	0.193668
a10	0			
a11	0			
a12	0			
a13	0			
a14	0			
a15	0			
a16	0			
a17	0		a17 must be less than or equal to	0.00218571
a18	0			
a19	0			
a20	0			
a21	0		a21 must be less than or equal to	0.00410006
a22	0			
a23	0			
a24	0			
a25	0			

TABLE F-7. DELTA II COEFFICIENTS, CASE 1, LOWER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
LOWER CLOUD				
test case #1.				
On-pad abort, confined by ground surface, no air entrainment in liquid cloud				
Product Composition				
coefficient	value		comment	
b1	0.007017			
b2	0			
b3	0			
b4	0.112679			
b5	0.067769			
b6	0			
b7	0			
b8	0			
b9	0.10669			
b10	0			
b11	0.052376		b11 must be > or = to 0	
b12	0			
b13	0.043234			
b14	0			
b15	0			
b16	0			
b17	0			
b18	0			
b19	0			
b20	0.200678			
b21	0.084062			
b22	0.049843			
b23	0			
b24	0			
b25	0			
b26	0			
b27	0			
b28	0			
b29	0			
b30	0			
b31	0			
b32	0			
b33	0			
b34	0			
b35	0			
b36	0			
b37	0			
b38	0			

TABLE F-7. DELTA II COEFFICIENTS, CASE 1, LOWER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
LOWER CLOUD				
test case #1.				
On-pad abort, confined by ground surface, no air entrainment in liquid cloud				
SUMMARY				
Consumed	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
O2(l)	0	#DIV/0!	0	31.999
RP-1(l)	0	#DIV/0!	0	13.976
NH4ClO4(s)	0	#DIV/0!	0	117.489
CH1.622(s)	0	#DIV/0!	0	13.646
Al(s)	0	#DIV/0!	0	26.982
Total	0			
REACTANTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
NH4ClO4	0.08685	15.35529	145450	117.489
CH1.622	0.12069	21.33829	23476	13.646
Al	0.10404	18.39453	40015	26.982
O2(l)	0	0	0	31.999
O2(g)	0.053345	9.431483	24332	31.999
N2	0.200678	35.48034	80132	28.013
RP-1	0	0	0	13.976
N2O4	0	0	0	92.016
UDMH	0	0	0	60.102
N2H4	0	0	0	32.045
Total	0.565603	99.99993	313404	
PRODUCTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
CO2	0.007017	0.968798	4402	44.01
CO	0.112679	15.55593	44989	28.01
H2O	0.174459	24.08488	44799	18.015
H2	0.052376	7.230806	1505	2.016
N2	0.243912	33.67324	97395	28.013
HCl	0.084062	11.6052	43689	36.461
Al2O3	0.049843	6.881105	72441	101.961
NO	0	0	0	30.006
O2	0	0	0	31.999
NH3	0	0	0	17.03
N2H4(g)	0	0	0	32.045
CH4	0	0	0	16.043
UDMH(g)	0	0	0	60.102
C2H4	0	0	0	28.054
C12H26(g)	0	0	0	170.337
N2O4(g)	0	0	0	92.016
NO2	0	0	0	46.006
HNO3	0	0	0	63.013
NOCl	0	0	0	65.451
Total	0.724349	99.99995	309221	

TABLE F-7. DELTA II COEFFICIENTS, CASE 1, LOWER CLOUD (CONCLUDED).

DELTA II SOURCE TERM MODEL	
REACTANT AND PRODUCT COMPOSITIONS	
LOWER CLOUD	
test case #1.	
On-pad abort, confined by ground surface, no air entrainment in liquid cloud	
Adiabatic Flame Temperature, K	3807
Average Molecular Weight (all products), lbs/lb-mole	29.95
Average Molecular Weight (gas products only), lbs/lb-mole	24.63
Fireball Diameter, empirical, feet	492
Fireball Volume, empirical, cubic feet	6.2545E+07
Fireball Diameter, ideal gas, feet	451
Fireball Volume, ideal gas, cubic feet	4.8099E+07
Total Heat Release, calories	-1.8052E+11

TABLE F-8. DELTA II THERMAL PROPERTIES, CASE 1, LOWER CLOUD.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #1 (lower cloud)

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.08685	NH4ClO4(s)	-70690						
0.12069	CH1.622(s)	-4241						
0.10404	Al(s)	0						
0	O2(l)	-3124						
0.053345	O2(g)	0						
0	CH1.95	-6220						
0	N2O4(l)	-4676						
0	UDMH(l)	12339						
0	N2H4(l)	12054						
0.200678	N2(g)	0						
0.007017	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.112679	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.174459	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0.052376	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
0.243912	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0.084062	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0.049843	Al2O3(l)	-381150	2315-5000	3.4620E+01	0.0000E+00	0.0000E+00	0.0000E+00	-1.0320E+04
0	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
0	C2H4(g)	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
0	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0	HNO3(g)	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
0	NOCl(g)	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
0	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0	C12H26(g)	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04

TABLE F-8. DELTA II THERMAL PROPERTIES, CASE 1, LOWER CLOUD (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #1 (lower cloud)

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K) A	B	C	D	E
NH4ClO4(s)	-6139.4265						
CH1.622(s)	-511.84629						
Al(s)	0						
O2(l)	0						
O2(g)	0						
CH1.95	0						
N2O4(l)	0						
UDMH(l)	0						
N2H4(l)	0						
N2(g)	0						
CO2	-659.962884	273-3700	4.4860E-02	7.0872E-05	-2.3893E-08	0.0000E+00	-1.6308E+01
CO	-2976.528464	273-3700	7.3016E-01	1.7646E-04	-2.6930E-08	0.0000E+00	-2.2513E+02
H2O	-10083.38128	273-3700	1.2160E+00	6.0433E-04	-8.4438E-08	0.0000E+00	-3.8852E+02
H2	0	273-3700	3.3646E-01	5.4419E-05	-4.0853E-09	0.0000E+00	-1.0266E+02
N2	0	273-3700	1.5925E+00	3.6294E-04	-5.5368E-08	0.0000E+00	-4.9026E+02
HCl	-1854.575844	1000-5000	4.6217E-01	2.4025E-04	-7.8514E-08	1.2281E-11	-1.4770E+02
Al2O3(s)	0	1000-2315	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Al2O3(l)	-18997.65945	2315-5000	1.7256E+00	0.0000E+00	0.0000E+00	0.0000E+00	-5.1438E+02
NO	0	273-3700	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
O2	0	273-3700	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NH3	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
CH4	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO2(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
HNO3(g)	0	0-1000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NOCl(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
UDMH(g)	0	0-2000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C12H26(g)	0	>270	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

TABLE F-8. DELTA II THERMAL PROPERTIES, CASE 1, LOWER CLOUD (CONCLUDED).

FIREBALL THERMAL PROPERTIES
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #1 (lower cloud)

A	B/2	C/3	D/4	E
6.1077E+00	7.5463E-04	-9.1076E-08	3.0704E-12	-1.8850E+03

HEAT OF FORMATION, REACTANTS (calories)	-6651.27279
HEAT OF FORMATION, PRODUCTS (calories)	-34572.1079
HEAT OF REACTION, (calories)	-27920.8351
FLAME TEMPERATURE (K)	3807

ΔHr+AT+B/2T^2+C/3T^3+D/4T^4+E
3.022075843

TABLE F-9. DELTA II COEFFICIENTS, CASE 2, UPPER CLOUD.

DELTA II SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
UPPER CLOUD		
test case #2		
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)		
Variable	Description	Value
s	Time of Abort (from launch), seconds	25
A	Altitude at Abort, feet	5000
α	Fraction Total Liquids in Cloud	1
β	Fraction Total Solids in Cloud	0.05
δ	Solid Propellant Reactivity Ratio	1
$\delta*$	Solid Propellant Consumption Ratio	0.74483
γl	Liquid Propellant Reactivity Ratio, LOX/RP-1	0.44
$\gamma l*$	Liquid Propellant Consumption Ratio, LOX/RP-1	0.90816
γ	Liquid Propellant Reactivity Ratio, N2O4/A-50	0.232
$\gamma*$	Liquid Propellant Consumption Ration, N2O4/A-50	1
ζ	Air Entrainment Ratio, Liquids	0.28756
ε	Fraction Excess Hydrazine Monodecomposed	0.7
η	Fraction Excess Hydrazine Vaporized	0.3
ξ	Fraction Excess UDMH Thermally Decomposed	0.5
ι	Fraction Excess UDMH Vaporized	0.5
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.1
μ	Fraction Excess RP-1 Thermall Decomposed (cracking)	0.5
υ	Fraction Excess RP-1 Vaporized	0.5
π	Fraction of Solids which Entrain Air	0
ρ	Air Entrainment Ratio, Solids	10.928
σ	HCl Reactivity	1
SF	Scaling Factor	6.4702E+06

TABLE F-9. DELTA II COEFFICIENTS, CASE 2, UPPER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
UPPER CLOUD				
test case #2				
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)				
Reactant Composition				
coefficient	value		comments	
a1	0.003594			
a2	0.004994			
a3	0.004305			
a4	0.036791			
a5	0			
a6	0.138406			
a7	0			
a8	0.127989			
a9	0.011883		a9 must be less than or equal to	0.17588153
a10	0.081999			
a11	0.081999			
a12	0.001554			
a13	0.001797			
a14	0.000335			
a15	0.003014			
a16	0.000527			
a17	9.66E-05		a17 must be less than or equal to	0.0021789
a18	0.001041			
a19	0.001041			
a20	0.000988			
a21	0.000184		a21 must be less than or equal to	0.00408728
a22	0.002732			
a23	0.001171			
a24	0.127989			
a25	0.162895			

TABLE F-9. DELTA II COEFFICIENTS, CASE 2, UPPER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
UPPER CLOUD				
test case #2				
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)				
Product Composition				
coefficient	value		comment	
b1	0.043428			
b2	0.000193			
b3	0.011883			
b4	0.090572			
b5	0.092236			
b6	0.000368			
b7	0.000386			
b8	0.011883			
b9	0			
b10	0.042659			
b11	0.006582		b11 must be > or = to 0	
b12	0.001366			
b13	0.004805			
b14	0.001366			
b15	0.000184			
b16	0.001041			
b17	9.66E-05			
b18	0.000335			
b19	0.138406			
b20	0			
b21	0.001739			
b22	0.002062			
b23	0.000116			
b24	0.000226			
b25	0.162895			
b26	0			
b27	0.018396			
b28	0.00067			
b29	0.002732			
b30	0.001171			
b31	0.002082			
b32	0.001041			
b33	0.041			
b34	0.006833			
b35	0			
b36	0.006028			
b37	0.001797			
b38	0.001797			

TABLE F-9. DELTA II COEFFICIENTS, CASE 2, UPPER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
UPPER CLOUD				
test case #2				
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)				
SUMMARY				
Consumed	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
O2(l)	0.029416	31.99481	13427	31.999
RP-1(l)	0.03073	33.42324	6126	13.976
NH4ClO4(s)	0.008863	9.639399	14853	117.489
CH1.622(s)	0.012316	13.39527	2397	13.646
Al(s)	0.010617	11.5473	4086	26.982
Total	0.091941	100	40890	
REACTANTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
NH4ClO4	0.003594	0.450732	6023	117.489
CH1.622	0.004994	0.626354	972	13.646
Al	0.004305	0.539944	1657	26.982
O2(l)	0.290884	36.4824	132773	31.999
O2(g)	0.036791	4.614347	16793	31.999
N2	0.138406	17.35873	55305	28.013
RP-1	0.30387	38.11118	60579	13.976
N2O4	0.0067	0.840309	8794	92.016
UDMH	0.002706	0.339384	2320	60.102
N2H4	0.005076	0.636578	2320	32.045
Total	0.797326	99.99996	287537	
PRODUCTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**
CO2	0.055504	7.947636	34844	44.01
CO	0.090572	12.96895	36188	28.01
H2O	0.104874	15.01678	26950	18.015
H2	0.050607	7.246367	1455	2.016
N2	0.146233	20.93904	58433	28.013
HCl	0.001739	0.249038	905	36.461
Al2O3	0.002062	0.295326	3000	101.961
NO	0.000116	0.016582	50	30.006
O2	0.182187	26.08729	83159	31.999
NH3	0.002732	0.391241	664	17.03
N2H4(g)	0.001171	0.167675	535	32.045
CH4	0.002082	0.298166	477	16.043
UDMH(g)	0.001041	0.149083	893	60.102
C2H4	0.041	5.870706	16407	28.054
C12H26(g)	0.006833	0.978412	16603	170.337
N2O4(g)	0	0	0	92.016
NO2	0.006028	0.863096	3956	46.006
HNO3	0.001797	0.257297	1615	63.013
NOCl	0.001797	0.257297	1678	65.451
Total	0.698376	99.99999	287809	

TABLE F-9. DELTA II COEFFICIENTS, CASE 2, UPPER CLOUD (CONCLUDED).

DELTA II SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
UPPER CLOUD		
test case #2		
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)		
Adiabatic Flame Temperature, K		1790
Average Molecular Weight (all products), lbs/lb-mole		28.89
Average Molecular Weight (gas products only), lbs/lb-mole		28.67
Fireball Diameter, empirical, feet		497
Fireball Volume, empirical, cubic feet		6.4458E+07
Fireball Diameter, ideal gas, feet		355
Fireball Volume, ideal gas, cubic feet		2.3364E+07
Total Heat Release, calories		-7.4377E+10

TABLE F-10. DELTA II THERMAL PROPERTIES, CASE 2, UPPER CLOUD.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #2 (upper cloud)

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.003594	NH4ClO4(s)	-70690						
0.004994	CH1.622(s)	-4241						
0.004305	Al(s)	0						
0.290884	O2(l)	-3124						
0.036791	O2(g)	0						
0.30387	CH1.95	-6220						
0.0067	N2O4(l)	-4676						
0.002706	UDMH(l)	12339						
0.005076	N2H4(l)	12054						
0.138406	N2(g)	0						
0.055504	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.090572	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.104874	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0.050607	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
0.146233	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0.001739	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0.002062	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0.000116	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0.182187	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0.002732	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0.002082	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
0.041	C2H4(g)	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
0.006028	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0.001797	HNO3(g)	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
0.001797	NOCl(g)	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
0.001171	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0.001041	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0.006833	C12H26(g)	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04

TABLE F-10. DELTA II THERMAL PROPERTIES, CASE 2, UPPER CLOUD (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #2 (upper cloud)

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K) A	B	C	D	E
NH4ClO4(s)	-254.05986						
CH1.622(s)	-21.179554						
Al(s)	0						
O2(l)	-908.721616						
O2(g)	0						
CH1.95	-1890.0714						
N2O4(l)	-31.3292						
UDMH(l)	33.389334						
N2H4(l)	61.186104						
N2(g)	0						
CO2	-5220.262208	273-3700	3.5484E-01	5.6059E-04	-1.8899E-07	0.0000E+00	-1.2899E+02
CO	-2392.549952	273-3700	5.8691E-01	1.4184E-04	-2.1647E-08	0.0000E+00	-1.8096E+02
H2O	-6061.507452	273-3700	7.3097E-01	3.6328E-04	-5.0759E-08	0.0000E+00	-2.3355E+02
H2	0	273-3700	3.2510E-01	5.2581E-05	-3.9473E-09	0.0000E+00	-9.9190E+01
N2	0	273-3700	9.5476E-01	2.1759E-04	-3.3195E-08	0.0000E+00	-2.9393E+02
HCl	-38.365818	1000-5000	9.5610E-03	4.9701E-06	-1.6242E-09	2.5407E-13	-3.0554E+00
Al2O3(s)	-825.831	1000-2315	5.1383E-02	1.0850E-05	-4.6106E-12	-1.0408E-12	-1.5799E+01
NO	2.5056	273-3700	7.4959E-04	2.7353E-07	-8.9320E-11	1.0127E-14	-2.3478E-01
O2	0	273-3700	1.2265E+00	2.7419E-04	-3.2811E-08	0.0000E+00	-3.7731E+02
NH3	-30.16128	273-1500	1.7993E-02	1.6736E-05	6.4639E-09	-4.3657E-12	-6.1552E+00
CH4	-37.244898	1000-5000	6.2173E-03	4.3099E-05	-1.6185E-08	2.8042E-12	-3.6291E+00
C2H4(g)	512.336	1000-5000	2.8151E-01	9.3632E-04	-3.5563E-07	6.2049E-11	-1.2245E+02
NO2(g)	47.98288	273-1500	3.3039E-02	8.2342E-05	-5.0756E-08	1.1333E-11	-1.3081E+01
HNO3(g)	-58.00716	0-1000	1.7246E-02	2.4655E-05	-9.0731E-09	0.0000E+00	-6.1529E+00
NOCl(g)	22.21092	1000-5000	1.9354E-02	6.4764E-06	-2.3882E-09	4.3919E-13	-6.0343E+00
N2H4(g)	26.270214	1000-5000	1.1851E-02	2.1664E-05	-7.8223E-09	1.3103E-12	-4.4264E+00
UDMH(g)	21.553905	0-2000	4.2265E-03	6.8081E-05	-2.2694E-08	0.0000E+00	-4.0818E+00
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C12H26(g)	-475.071158	>270	3.5275E-02	1.7526E-03	-9.3434E-07	1.9290E-10	-8.0472E+01

TABLE F-10. DELTA II THERMAL PROPERTIES, CASE 2, UPPER CLOUD (CONCLUDED).

FIREBALL THERMAL PROPERTIES
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #2 (upper cloud)

A	B/2	C/3	D/4	E
4.6675E+00	2.2891E-03	-5.7510E-07	6.6422E-11	-1.5795E+03

HEAT OF FORMATION, REACTANTS (calories)	-3010.78619
HEAT OF FORMATION, PRODUCTS (calories)	-14506.1414
HEAT OF REACTION, (calories)	-11495.3552
FLAME TEMPERATURE (K)	1790

ΔHr+AT+B/2T^2+C/3T^3+D/4T^4+E
-2.124907601

TABLE F-11. DELTA II COEFFICIENTS, CASE 2, LOWER CLOUD.

DELTA II SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
LOWER CLOUD		
test case #2		
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)		
Variable	Description	Value
s	Time of Abort (from launch), seconds	25
A	Altitude at Abort, feet	5000
α	Fraction Total Liquids in Cloud	0
β	Fraction Total Solids in Cloud	0.95
δ	Solid Propellant Reactivity Ratio	1
δ*	Solid Propellant Consumption Ratio	0.74483
γl	Liquid Propellant Reactivity Ratio, LOX/RP-1	0.44
γl*	Liquid Propellant Consumption Ratio, LOX/RP-1	0.90816
γ	Liquid Propellant Reactivity Ratio, N2O4/A-50	0.232
γ*	Liquid Propellant Consumption Ration, N2O4/A-50	1
ζ	Air Entrainment Ratio, Liquids	0.28756
ε	Fraction Excess Hydrazine Monodecomposed	0.7
η	Fraction Excess Hydrazine Vaporized	0.3
ξ	Fraction Excess UDMH Thermally Decomposed	0.5
ι	Fraction Excess UDMH Vaporized	0.5
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.1
μ	Fraction Excess RP-1 Thermall Decomposed (cracking)	0.5
υ	Fraction Excess RP-1 Vaporized	0.5
π	Fraction of Solids which Entrain Air	1
ρ	Air Entrainment Ratio, Solids	10.92810339
σ	HCl Reactivity	0
SF	Scaling Factor	6.4656E+06

TABLE F-11. DELTA II COEFFICIENTS, CASE 2, LOWER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
LOWER CLOUD				
test case #2				
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)				
Reactant Composition				
coefficient	value		comments	
a1	0.068282			
a2	0.094888			
a3	0.081797			
a4	0			
a5	0.156701			
a6	0			
a7	0.589495			
a8	0			
a9	0		a9 must be less than or equal to	0.175881531
a10	0			
a11	0			
a12	0			
a13	0			
a14	0			
a15	0			
a16	0			
a17	0		a17 must be less than or equal to	0.002178896
a18	0			
a19	0			
a20	0			
a21	0		a21 must be less than or equal to	0.00408728
a22	0			
a23	0			
a24	0			
a25	0			

TABLE F-11. DELTA II COEFFICIENTS, CASE 2, LOWER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
LOWER CLOUD				
test case #2				
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)				
Product Composition				
coefficient	value		comment	
b1	0.005517			
b2	0			
b3	0			
b4	0.088589			
b5	0.053281			
b6	0			
b7	0			
b8	0			
b9	0.125059			
b10	0			
b11	0		b11 must be > or = to 0 (was -0.17159, changed to 0)	
b12	0			
b13	0.033991			
b14	0			
b15	0			
b16	0			
b17	0			
b18	0			
b19	0			
b20	0.589495			
b21	0.06609			
b22	0.039187			
b23	0			
b24	0			
b25	0			
b26	0.094172			
b27	0			
b28	0			
b29	0			
b30	0			
b31	0			
b32	0			
b33	0			
b34	0			
b35	0			
b36	0			
b37	0			
b38	0			

TABLE F-11. DELTA II COEFFICIENTS, CASE 2, LOWER CLOUD (CONTINUED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
LOWER CLOUD				
test case #2				
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)				
SUMMARY				
Consumed	g-mole	mole %	Mass, Lb	Mol. Wt.
O2(l)	0.029416	31.99481	13417	31.999
RP-1(l)	0.03073	33.42324	6122	13.976
NH4ClO4(s)	0.008863	9.639399	14842	117.489
CH1.622(s)	0.012316	13.39527	2396	13.646
Al(s)	0.010617	11.5473	4083	26.982
Total	0.091941	100	40861	
REACTANTS	g-mole	mole %	Mass, Lb	Mol. Wt.
NH4ClO4	0.068282	6.889108	114354	117.489
CH1.622	0.094888	9.573362	18457	13.646
Al	0.081797	8.252652	31460	26.982
O2(l)	0	0	0	31.999
O2(g)	0.156701	15.80983	71475	31.999
N2	0.589495	59.47506	235388	28.013
RP-1	0	0	0	13.976
N2O4	0	0	0	92.016
UDMH	0	0	0	60.102
N2H4	0	0	0	32.045
Total	0.991163	100	471134	
PRODUCTS	g-mole	mole %	Mass, Lb	Mol. Wt.
CO2	0.005517	0.503679	3461	44.01
CO	0.088589	8.087546	35370	28.01
H2O	0.17834	16.28106	45796	18.015
H2	0	0	0	2.016
N2	0.623486	56.91953	248961	28.013
HCl	0.06609	6.033556	34349	36.461
Al2O3	0.039187	3.577496	56954	101.961
NO	0	0	0	30.006
O2	0.094172	8.597158	42954	31.999
NH3	0	0	0	17.03
N2H4(g)	0	0	0	32.045
CH4	0	0	0	16.043
UDMH(g)	0	0	0	60.102
C2H4	0	0	0	28.054
C12H26(g)	0	0	0	170.337
N2O4(g)	0	0	0	92.016
NO2	0	0	0	46.006
HNO3	0	0	0	63.013
NOCl	0	0	0	65.451
Total	1.095381	100	467845	

TABLE F-11. DELTA II COEFFICIENTS, CASE 2, LOWER CLOUD (CONCLUDED).

DELTA II SOURCE TERM MODEL				
REACTANT AND PRODUCT COMPOSITIONS				
LOWER CLOUD				
test case #2				
Abort at 5000 ft, Command Destruct, 35% Air Entrainment Liquids (lb/lb)				
Adiabatic Flame Temperature, K				2625
Average Molecular Weight (all products), lbs/lb-mole				29.96
Average Molecular Weight (gas products only), lbs/lb-mole				27.29
Fireball Diameter, empirical, feet				455
Fireball Volume, empirical, cubic feet				4.9363E+07
Fireball Diameter, ideal gas, feet				463
Fireball Volume, ideal gas, cubic feet				5.1933E+07
Total Heat Release, calories				-1.5732E+11

TABLE F-12. DELTA II THERMAL PROPERTIES, CASE 2, LOWER CLOUD.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #2 (lower cloud)

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.068282	NH4ClO4(s)	-70690						
0.094888	CH1.622(s)	-4241						
0.081797	Al(s)	0						
0	O2(l)	-3124						
0.156701	O2(g)	0						
0	CH1.95	-6220						
0	N2O4(l)	-4676						
0	UDMH(l)	12339						
0	N2H4(l)	12054						
0.589495	N2(g)	0						
0.005517	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.088589	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.17834	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
0.623486	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0.06609	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0.039187	Al2O3(l)	-381150	2315-5000	3.4620E+01	0.0000E+00	0.0000E+00	0.0000E+00	-1.0320E+04
0	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0.094172	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
0	C2H4(g)	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
0	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0	HNO3(g)	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
0	NOCl(g)	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
0	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0	C12H26(g)	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04

TABLE F-12. DELTA II THERMAL PROPERTIES, CASE 2, LOWER CLOUD (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #2 (lower cloud)

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K) A	B	C	D	E
NH4ClO4(s)	-4826.85458						
CH1.622(s)	-402.420008						
Al(s)	0						
O2(l)	0						
O2(g)	0						
CH1.95	0						
N2O4(l)	0						
UDMH(l)	0						
N2H4(l)	0						
N2(g)	0						
CO2	-518.884884	273-3700	3.5270E-02	5.5722E-05	-1.8785E-08	0.0000E+00	-1.2822E+01
CO	-2340.167024	273-3700	5.7406E-01	1.3873E-04	-2.1173E-08	0.0000E+00	-1.7700E+02
H2O	-10307.69532	273-3700	1.2430E+00	6.1777E-04	-8.6317E-08	0.0000E+00	-3.9716E+02
H2	0	273-3700	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2	0	273-3700	4.0707E+00	9.2775E-04	-1.4153E-07	0.0000E+00	-1.2532E+03
HCl	-1458.07758	1000-5000	3.6336E-01	1.8889E-04	-6.1728E-08	9.6557E-12	-1.1612E+02
Al2O3(s)	0	1000-2315	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Al2O3(l)	-14936.12505	2315-5000	1.3567E+00	0.0000E+00	0.0000E+00	0.0000E+00	-4.0441E+02
NO	0	273-3700	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
O2	0	273-3700	6.3397E-01	1.4173E-04	-1.6857E-08	0.0000E+00	-1.9503E+02
NH3	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
CH4	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO2(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
HNO3(g)	0	0-1000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NOCl(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
UDMH(g)	0	0-2000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C12H26(g)	0	>270	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

TABLE F-12. DELTA II THERMAL PROPERTIES, CASE 2, LOWER CLOUD (CONCLUDED).

FIREBALL THERMAL PROPERTIES
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: DELTA II MODEL test case #2 (lower cloud)

A	B/2	C/3	D/4	E
8.2771E+00	1.0353E-03	-1.1546E-07	2.4139E-12	-2.5558E+03

HEAT OF FORMATION, REACTANTS (calories)	-5229.27459
HEAT OF FORMATION, PRODUCTS (calories)	-29560.9499
HEAT OF REACTION, (calories)	-24331.6753
FLAME TEMPERATURE (K)	2625

ΔHr+AT+B/2T^2+C/3T^3+D/4T^4+E
-0.166492407

TABLE F-13. TITAN IV COEFFICIENTS, CASE 1, UPPER CLOUD.

TITAN IV SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
UPPER CLOUD		
test case #1		
On Pad Abort, no air entrainment		
Variable	Description	Value
s	Time of Abort (from launch), seconds	0
A	Altitude at Abort, feet	0
α	Fraction Total Liquids in Cloud	1
β	Fraction Total Solids in Cloud	0.1
δ	Solid Propellant Reactivity Ratio	1
δ*	Solid Propellant Consumption Ratio	1
γ	Liquid Propellant Reactivity Ratio	0.229
γ*	Liquid Propellant Consumption Ratio	1
ζ	Air Entrainment Ratio, Liquids	0
ε	Fraction Excess Hydrazine Monodecomposed	0.94
η	Fraction Excess Hydrazine Vaporized	0.06
ξ	Fraction Excess UDMH Thermally Decomposed	0.7
ι	Fraction Excess UDMH Vaporized	0.3
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.35
π	Fraction of Solids which Entrain Air	0
ρ	Air Entrainment Ratio, Solids	3.0161524
σ	HCl Reactivity	1
SF	Scaling Factor	1.4988E+07

TABLE F-13. TITAN IV COEFFICIENTS, CASE 1, UPPER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
UPPER CLOUD					
test case #1					
On Pad Abort, no air entrainment					
Reactant Composition					
coefficient	value		comments		
a1	0.02055				
a2	0.03777				
a3	0.02137				
a4	5.59E-05				
a5	0				
a6	0				
a7	0				
a8	0				
a9	0.02077				
a10	0.010275				
a11	0.022804				
a12	0.042351				
a13	0.007076				
a14	0		a14 must be less than or equal to	0.0299239	
a15	0.020947				
a16	0.008977				
a17	0.013259				
a18	0		a18 must be less than or equal to	0.0561409	
a19	0.052772				
a20	0.003368				

TABLE F-13. TITAN IV COEFFICIENTS, CASE 1, UPPER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
UPPER CLOUD					
test case #1					
On Pad Abort, no air entrainment					
Product Composition					
coefficient	value		comment		
b1	0.0082				
b2	0				
b3	0.043726				
b4	0.069103				
b5	0				
b6	0				
b7	0				
b8	0.0435		b8 must be > or = to 0		
b9	0.026386				
b10	0.050939				
b11	0.026386				
b12	0				
b13	0.020947				
b14	0				
b15	0.022804				
b16	0				
b17	0				
b18	0.01021				
b19	0.010546				
b20	0.001547				
b21	0.003024				
b22	0				
b23	0				
b24	0.045608				
b25	0.052772				
b26	0.003368				
b27	0.041893				
b28	0.008977				
b29	0				
b30	0.084701				
b31	0.010275				
b32	0.010275				
b33	5.59E-05				

TABLE F-13. TITAN IV COEFFICIENTS, CASE 1, UPPER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
UPPER CLOUD					
test case #1					
On Pad Abort, no air entrainment					
SUMMARY					
Consumed	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
NH4ClO4	0	0	0	117.489	
PBAN	0	0	0	15.263	
Al	0	0	0	26.982	
Total	0	0	0		
REACTANTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
NH4ClO4	0.02055	7.278304	79782	117.489	
PBAN	0.03777	13.3772	19049	15.263	
Al	0.02137	7.568728	19053	26.982	
Fe2O3	5.59E-05	0.019798	295	159.692	
O2	0	0	0	31.999	
N2	0	0	0	28.013	
N2O4	0.0962	34.07167	292504	92.016	
UDMH	0.037	13.10449	73483	60.102	
N2H4	0.0694	24.57977	73487	32.045	
Total	0.282346	99.99996	557654		
PRODUCTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
CO2	0.0082	1.377501	11924	44.01	
CO	0.043726	7.345891	40471	28.01	
H2O	0.069103	11.60918	41136	18.015	
H2	0.069886	11.74075	4656	2.016	
N2	0.121076	20.34053	112076	28.013	
HCl	0.01021	1.715299	12302	36.461	
Al2O3	0.010546	1.771745	35533	101.961	
NO	0.001547	0.259957	1534	30.006	
O2	0.048632	8.170129	51423	31.999	
NH3	0.052772	8.865638	29697	17.03	
N2H4(g)	0.003368	0.565892	3567	32.045	
CH4	0.041893	7.037996	22205	16.04	
UDMH(g)	0.008977	1.508142	17829	60.102	
N2O4(g)	0	0	0	92.016	
NO2	0.084701	14.22957	128765	46.006	
HNO3	0.010275	1.726174	21395	63.013	
NOCl	0.010275	1.726174	22225	65.459	
Fe2O3	5.59E-05	0.009391	295	159.692	
Total	0.595247	99.99996	557032		

TABLE F-13. TITAN IV COEFFICIENTS, CASE 1, UPPER CLOUD (CONCLUDED).

TITAN IV SOURCE TERM MODEL			
REACTANT AND PRODUCT COMPOSITIONS			
UPPER CLOUD			
test case #1			
On Pad Abort, no air entrainment			
Adiabatic Flame Temperature, K			1830
Average Molecular Weight (all products), lbs/lb-mole			28.32
Average Molecular Weight (gas products only), lbs/lb-mole			26.98
Fireball Diameter, empirical, feet			673
Fireball Volume, empirical, cubic feet			1.5948E+08
Fireball Diameter, ideal gas, feet			446
Fireball Volume, ideal gas, cubic feet			4.6459E+07
Total Heat Release, calories			-1.528E+11

TABLE F-14. TITAN IV THERMAL PROPERTIES, CASE 1, UPPER CLOUD.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #1 upper cloud

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.02055	NH4ClO4(s)	-70690						
0.03777	PBAN*	-3434						
0.02137	Al(s)	0						
0.00006	Fe2O3(s)	-197000						
0	O2(l)	-3124						
0	O2(g)	0						
0	CH1.95	-6220						
0.0962	N2O4(l)	-4676						
0.037	UDMH(l)	12339						
0.0694	N2H4(l)	12054						
0	N2(g)	0						
0.0082	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.043726	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.069103	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0.069886	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
0.121076	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0.01021	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0	Al2O3(l)**	-381150	2315-5000	3.4620E+01	0.0000E+00	0.0000E+00	0.0000E+00	-1.0320E+04
0.010546	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0.001547	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0.048632	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0.052772	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0.041893	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
0	C2H4(g)	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
0.084701	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0.010275	HNO3(g)	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
0.010275	NOCl(g)	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
0.003368	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0.008977	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0	C12H26(g)	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04
0.00006	Fe2O3(s)	-197000	1000-2500	8.0480E+01	-9.1670E-02	6.3250E-05	-1.3760E-08	-2.0440E+04

*Note: Empirical Formula for PBAN is C H1.427 O.095 N.021; This formula and thermal properties are different than PBAN used for T34D Modeling

TABLE F-14. TITAN IV THERMAL PROPERTIES, CASE 1, UPPER CLOUD (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #1 upper cloud

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K) A	B	C	D	E
NH4ClO4(s)	-1452.6795						
PBAN	-129.70218						
Al(s)	0						
Fe2O3(s)	-11.82						
O2(l)	0						
O2(g)	0						
CH1.95	0						
N2O4(l)	-449.8312						
UDMH(l)	456.543						
N2H4(l)	836.5476						
N2(g)	0						
CO2	-771.2264	273-3700	5.2423E-02	8.2820E-05	-2.7921E-08	0.0000E+00	-1.9057E+01
CO	-1155.066016	273-3700	2.8334E-01	6.8475E-05	-1.0451E-08	0.0000E+00	-8.7365E+01
H2O	-3994.015194	273-3700	4.8165E-01	2.3937E-04	-3.3446E-08	0.0000E+00	-1.5389E+02
H2	0	273-3700	4.4895E-01	7.2612E-05	-5.4511E-09	0.0000E+00	-1.3698E+02
N2	0	273-3700	7.9051E-01	1.8016E-04	-2.7484E-08	0.0000E+00	-2.4336E+02
HCl	-225.25302	1000-5000	5.6135E-02	2.9180E-05	-9.5361E-09	1.4917E-12	-1.7939E+01
Al2O3(l)	0	2615-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Al2O3(s)	-4223.673	1000-2315	2.6280E-01	5.5493E-05	-2.3581E-11	-5.3231E-12	-8.0803E+01
NO	33.4152	273-3700	9.9967E-03	3.6478E-06	-1.1912E-09	1.3505E-13	-3.1311E+00
O2	0	273-3700	3.2739E-01	7.3191E-05	-8.7051E-09	0.0000E+00	-1.0072E+02
NH3	-582.60288	273-1500	3.4756E-01	3.2328E-04	1.2486E-07	-8.4330E-11	-1.1890E+02
CH4	-749.423877	1000-5000	1.2510E-01	8.6723E-04	-3.2568E-07	5.6426E-11	-7.3024E+01
C2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO2(g)	674.21996	273-1500	4.6425E-01	1.1570E-03	-7.1318E-07	1.5924E-10	-1.8380E+02
HNO3(g)	-331.677	0-1000	9.8609E-02	1.4097E-04	-5.1878E-08	0.0000E+00	-3.5182E+01
NOCl(g)	126.999	1000-5000	1.1066E-01	3.7031E-05	-1.3655E-08	2.5112E-12	-3.4503E+01
N2H4(g)	75.557712	1000-5000	3.4084E-02	6.2308E-05	-2.2498E-08	3.7688E-12	-1.2731E+01
UDMH(g)	185.868785	0-2000	3.6447E-02	5.8710E-04	-1.9570E-07	0.0000E+00	-3.5199E+01
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C12H26(g)	0	>270	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Fe2O3(s)	-11.82	1000-2500	4.8288E-03	-5.5002E-06	3.7950E-09	-8.2560E-13	-1.2264E+00

TABLE F-14. TITAN IV THERMAL PROPERTIES, CASE 1, UPPER CLOUD (CONCLUDED).

FIREBALL THERMAL PROPERTIES
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #1 upper cloud

A	B/2	C/3	D/4	E
3.9347E+00	1.9872E-03	-4.3938E-07	3.3273E-11	-1.3378E+03

HEAT OF FORMATION, REACTANTS (calories)	-750.94228
HEAT OF FORMATION, PRODUCTS (calories)	-10948.6967
HEAT OF REACTION, (calories)	-10197.7545
FLAME TEMPERATURE (K)	1830

ΔH+AT+B/2T^2+C/3T^3+D/4T^4+E
0.301793888

TABLE F-15. TITAN IV COEFFICIENTS, CASE 1, LOWER CLOUD.

TITAN IV SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
LOWER CLOUD		
test case #1.		
On Pad Abort, no air entrainment		
Variable	Description	Value
s	Time of Abort (from launch), seconds	0
A	Altitude at Abort, feet	0
α	Fraction Total Liquids in Cloud	0
β	Fraction Total Solids in Cloud	0.9
δ	Solid Propellant Reactivity Ratio	1
$\delta*$	Solid Propellant Consumption Ratio	1
γ	Liquid Propellant Reactivity Ratio	0.229
$\gamma*$	Liquid Propellant Consumption Ratio	1
ζ	Air Entrainment Ratio, Liquids	0
ε	Fraction Excess Hydrazine Monodecomposed	0.94
η	Fraction Excess Hydrazine Vaporized	0.06
ξ	Fraction Excess UDMH Thermally Decomposed	0.7
ι	Fraction Excess UDMH Vaporized	0.3
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.35
π	Fraction of Solids which Entrain Air	1
ρ	Air Entrainment Ratio, Solids	3.0161524
σ	HCl Reactivity	0
SF	Scaling Factor	1.4991E+07

TABLE F-15. TITAN IV COEFFICIENTS, CASE 1, LOWER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
LOWER CLOUD					
test case #1.					
On Pad Abort, no air entrainment					
Reactant Composition					
coefficient	value		comments		
a1	0.18495				
a2	0.33993				
a3	0.19233				
a4	0.000503				
a5	0				
a6	0.117146				
a7	0				
a8	0.440692				
a9	0				
a10	0				
a11	0				
a12	0				
a13	0				
a14	0		a14 must be less than or equal to	0.0299239	
a15	0				
a16	0				
a17	0				
a18	0		a18 must be less than or equal to	0.0561409	
a19	0				
a20	0				

TABLE F-15. TITAN IV COEFFICIENTS, CASE 1, LOWER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
LOWER CLOUD					
test case #1.					
On Pad Abort, no air entrainment					
Product Composition					
coefficient	value		comment		
b1	0.016183				
b2	0				
b3	0.323866				
b4	0.128633				
b5	0				
b6	0				
b7	0.2342917				
b8	0.15721		b8 must be > or = to 0		
b9	0				
b10	0.095767				
b11	0				
b12	0				
b13	0				
b14	0				
b15	0				
b16	0				
b17	0.440692				
b18	0.183785				
b19	0.094916				
b20	0				
b21	0				
b22	0				
b23	0				
b24	0				
b25	0				
b26	0				
b27	0				
b28	0				
b29	0				
b30	0				
b31	0				
b32	0				
b33	0.000503				

TABLE F-15. TITAN IV COEFFICIENTS, CASE 1, LOWER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
LOWER CLOUD					
test case #1.					
On Pad Abort, no air entrainment					
SUMMARY					
Consumed	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
NH4ClO4	0	#DIV/0!	0	117.489	
PBAN	0	#DIV/0!	0	15.263	
Al	0	#DIV/0!	0	26.982	
Total	0	#DIV/0!	0		
REACTANTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
NH4ClO4	0.18495	14.52618	718156	117.489	
PBAN	0.33993	26.69849	171473	15.263	
Al	0.19233	15.10582	171510	26.982	
Fe2O3	0.000503	0.039514	2655	159.692	
O2	0.117146	9.200769	123888	31.999	
N2	0.440692	34.61242	408001	28.013	
N2O4	0	0	0	92.016	
UDMH	0	0	0	60.102	
N2H4	0	0	0	32.045	
Total	1.27555	100.18320	1595683		
PRODUCTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
CO2	0.016183	0.966732	23539	44.01	
CO	0.323866	19.34678	299810	28.01	
H2O	0.362924	21.68002	216082	18.015	
H2	0.15721	9.391283	10475	2.016	
N2	0.536459	32.04644	496664	28.013	
HCl	0.183785	10.97876	221465	36.461	
Al2O3	0.094916	5.670019	319847	101.961	
NO	0	0	0	30.006	
O2	0	0	0	31.999	
NH3	0	0	0	17.03	
N2H4(g)	0	0	0	32.045	
CH4	0	0	0	16.04	
UDMH(g)	0	0	0	60.102	
N2O4(g)	0	0	0	92.016	
NO2	0	0	0	46.006	
HNO3	0	0	0	63.013	
NOCl	0	0	0	65.459	
Fe2O3	0.000503	0.030054	2655	159.692	
Total	1.675847	100.11009	1590536		

TABLE F-15. TITAN IV COEFFICIENTS, CASE 1, LOWER CLOUD (CONCLUDED).

TITAN IV SOURCE TERM MODEL			
REACTANT AND PRODUCT COMPOSITIONS			
LOWER CLOUD			
test case #1.			
On Pad Abort, no air entrainment			
Adiabatic Flame Temperature, K			3534
Average Molecular Weight (all products), lbs/lb-mole			28.72
Average Molecular Weight (gas products only), lbs/lb-mole			24.28
Fireball Diameter, empirical, feet			836
Fireball Volume, empirical, cubic feet			3.0546E+08
Fireball Diameter, ideal gas, feet			774
Fireball Volume, ideal gas, cubic feet			2.4257E+08
Total Heat Release, calories			-8.551E+11

TABLE F-16. TITAN IV THERMAL PROPERTIES, CASE 1, LOWER CLOUD.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #1 lower cloud

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.18495	NH4ClO4(s)	-70690						
0.33993	PBAN*	-3434						
0.19233	Al(s)	0						
0.000503	Fe2O3(s)	-197000						
0	O2(l)	-3124						
0.117117	O2(g)	0						
0	CH1.95	-6220						
0	N2O4(l)	-4676						
0	UDMH(l)	12339						
0	N2H4(l)	12054						
0.440583	N2(g)	0						
0.016183	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.323866	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.362867	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0.157268	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
0.53635	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0.183785	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0.094916	Al2O3(l)**	-381150	2315-5000	3.4620E+01	0.0000E+00	0.0000E+00	0.0000E+00	-1.0320E+04
0	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
0	C2H4(g)	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
0	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0	HNO3(g)	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
0	NOCl(g)	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
0	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0	C12H26(g)	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04
0.000503	Fe2O3(s)	-197000	1000-2500	8.0480E+01	-9.1670E-02	6.3250E-05	-1.3760E-08	-2.0440E+04

*Note: Empirical Formula for PBAN is C H1.427 O.095 N.021; This formula and thermal properties are different than PBAN used for T34D Modeling

TABLE F-16. TITAN IV THERMAL PROPERTIES, CASE 1, LOWER CLOUD (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #1 lower cloud

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K) A	B	C	D	E
NH4ClO4(s)	-13074.1155						
PBAN	-1167.31962						
Al(s)	0						
Fe2O3(s)	-99.091						
O2(l)	0						
O2(g)	0						
CH1.95	0						
N2O4(l)	0						
UDMH(l)	0						
N2H4(l)	0						
N2(g)	0						
CO2	-1522.043516	273-3700	1.0346E-01	1.6345E-04	-5.5103E-08	0.0000E+00	-3.7609E+01
CO	-8555.244256	273-3700	2.0987E+00	5.0717E-04	-7.7404E-08	0.0000E+00	-6.4708E+02
H2O	-20972.98687	273-3700	2.5292E+00	1.2570E-03	-1.7563E-07	0.0000E+00	-8.0810E+02
H2	0	273-3700	1.0103E+00	1.6340E-04	-1.2267E-08	0.0000E+00	-3.0825E+02
N2	0	273-3700	3.5018E+00	7.9809E-04	-1.2175E-07	0.0000E+00	-1.0781E+03
HCl	-4054.66467	1000-5000	1.0104E+00	5.2526E-04	-1.7166E-07	2.6851E-11	-3.2291E+02
Al2O3(l)	-36177.2334	2615-5000	3.2860E+00	0.0000E+00	0.0000E+00	0.0000E+00	-9.7953E+02
Al2O3(s)	0	1000-2315	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO	0	273-3700	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
O2	0	273-3700	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NH3	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
CH4	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO2(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
HNO3(g)	0	0-1000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NOCl(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
UDMH(g)	0	0-2000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C12H26(g)	0	>270	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Fe2O3(s)	-99.091	1000-2500	4.0481E-02	-4.6110E-05	3.1815E-08	-6.9213E-12	-1.0281E+01

TABLE F-16. TITAN IV THERMAL PROPERTIES, CASE 1, LOWER CLOUD (CONCLUDED).

FIREBALL THERMAL PROPERTIES
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #1 lower cloud

A	B/2	C/3	D/4	E
1.3580E+01	1.6841E-03	-1.9400E-07	4.9824E-12	-4.1918E+03

HEAT OF FORMATION, REACTANTS (calories)	-14340.5261
HEAT OF FORMATION, PRODUCTS (calories)	-71381.2637
HEAT OF REACTION, (calories)	-57040.7376
FLAME TEMPERATURE (K)	3534

ΔH+AT+B/2T^2+C/3T^3+D/4T^4+E
8.251852534

TABLE F-17. TITAN IV COEFFICIENTS, CASE 2, UPPER CLOUD.

TITAN IV SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
UPPER CLOUD		
test case #2		
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids		
Variable	Description	Value
s	Time of Abort (from launch), seconds	25
A	Altitude at Abort, feet	5000
α	Fraction Total Liquids in Cloud	1
β	Fraction Total Solids in Cloud	0.05
δ	Solid Propellant Reactivity Ratio	1
$\delta*$	Solid Propellant Consumption Ratio	0.772335
γ	Liquid Propellant Reactivity Ratio	0.232
$\gamma*$	Liquid Propellant Consumption Ratio	1
ζ	Air Entrainment Ratio, Liquids	0.35
ε	Fraction Excess Hydrazine Monodecomposed	0.7
η	Fraction Excess Hydrazine Vaporized	0.3
ξ	Fraction Excess UDMH Thermally Decomposed	0.5
ι	Fraction Excess UDMH Vaporized	0.5
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.1
π	Fraction of Solids which Entrain Air	0
ρ	Air Entrainment Ratio, Solids	5.095899
σ	HCl Reactivity	1
SF	Scaling Factor	1.4988E+07

TABLE F-17. TITAN IV COEFFICIENTS, CASE 2, UPPER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
UPPER CLOUD					
test case #2					
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids					
Reactant Composition					
coefficient	value		comments		
a1	0.007936				
a2	0.014586				
a3	0.008252				
a4	2.16E-05				
a5	0.014875				
a6	0				
a7	0.056035				
a8	0				
a9	0.021042				
a10	0.003968				
a11	0.007119				
a12	0.064071				
a13	0.007169				
a14	0.001488		a14 must be less than or equal to	0.0298312	
a15	0.014172				
a16	0.014172				
a17	0.013433				
a18	0.001488		a18 must be less than or equal to	0.0559672	
a19	0.038136				
a20	0.016344				

TABLE F-17. TITAN IV COEFFICIENTS, CASE 2, UPPER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
UPPER CLOUD					
test case #2					
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids					
Product Composition					
coefficient	value		comment		
b1	0.00718				
b2	0.002975				
b3	0.021739				
b4	0.061048				
b5	0.002975				
b6	0.00595				
b7	0				
b8	0.016798		b8 must be > or = to 0		
b9	0.019068				
b10	0.044936				
b11	0.019068				
b12	0.001488				
b13	0.014172				
b14	0.001488				
b15	0.007119				
b16	0.056035				
b17	0				
b18	0.003943				
b19	0.004073				
b20	0.001568				
b21	0.003064				
b22	0				
b23	0.007438				
b24	0.014238				
b25	0.038136				
b26	0.016344				
b27	0.028344				
b28	0.014172				
b29	0				
b30	0.128142				
b31	0.003968				
b32	0.003968				
b33	2.16E-05				

TABLE F-17. TITAN IV COEFFICIENTS, CASE 2, UPPER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
UPPER CLOUD					
test case #2					
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids					
SUMMARY					
Consumed	g-mole	mole %	Mass, Lb	Mol. Wt.	
NH4ClO4	0.046785	25.78746	181635	117.489	
PBAN	0.085989	47.39622	43369	15.263	
Al	0.048652	26.81645	43378	26.982	
Total	0.181426	100.0001	268381		
REACTANTS	g-mole	mole %	Mass, Lb	Mol. Wt.	
NH4ClO4	0.007936	2.607825	30809	117.489	
PBAN	0.014586	4.793068	7356	15.263	
Al	0.008252	2.711884	7358	26.982	
Fe2O3	2.16E-05	0.007094	114	159.692	
O2	0.014875	4.888188	15728	31.999	
N2	0.056035	18.41409	51870	28.013	
N2O4	0.0962	31.61302	292504	92.016	
UDMH	0.037	12.15885	73483	60.102	
N2H4	0.0694	22.80607	73487	32.045	
Total	0.304305	100.00009	552709		
PRODUCTS	g-mole	mole %	Mass, Lb	Mol. Wt.	
CO2	0.010155	1.848134	14768	44.01	
CO	0.021739	3.956433	20121	28.01	
H2O	0.069973	12.73502	41654	18.015	
H2	0.035866	6.527621	2389	2.016	
N2	0.144304	26.26322	133577	28.013	
HCl	0.003943	0.717598	4750	36.461	
Al2O3	0.004073	0.741213	13722	101.961	
NO	0.001568	0.285312	1554	30.006	
O2	0.024739	4.50251	26159	31.999	
NH3	0.038136	6.94067	21461	17.03	
N2H4(g)	0.016344	2.974573	17307	32.045	
CH4	0.028344	5.158521	15023	16.04	
UDMH(g)	0.014172	2.579261	28146	60.102	
N2O4(g)	0	0	0	92.016	
NO2	0.128142	23.32161	194804	46.006	
HNO3	0.003968	0.722148	8262	63.013	
NOCl	0.003968	0.722148	8583	65.459	
Fe2O3	2.16E-05	0.003929	114	159.692	
Total	0.549454	99.99992	552392		

TABLE F-17. TITAN IV COEFFICIENTS, CASE 2, UPPER CLOUD (CONCLUDED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
UPPER CLOUD					
test case #2					
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids					
Adiabatic Flame Temperature, K					1407
Average Molecular Weight (all products), lbs/lb-mole					30.42
Average Molecular Weight (gas products only), lbs/lb-mole					29.89
Fireball Diameter, empirical, feet					642
Fireball Volume, empirical, cubic feet					1.3841E+08
Fireball Diameter, ideal gas, feet					399
Fireball Volume, ideal gas, cubic feet					3.3320E+07
Total Heat Release, calories					-1.022E+11

TABLE F-18. TITAN IV THERMAL PROPERTIES, CASE 2, UPPER CLOUD.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #2 upper cloud

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.007936	NH4ClO4(s)	-70690						
0.014586	PBAN*	-3434						
0.008252	Al(s)	0						
2.16E-05	Fe2O3(s)	-197000						
0	O2(l)	-3124						
0.014875	O2(g)	0						
0	CH1.95	-6220						
0.0962	N2O4(l)	-4676						
0.037	UDMH(l)	12339						
0.0694	N2H4(l)	12054						
0.056035	N2(g)	0						
0.010155	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.021739	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.069973	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0.035866	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
0.144304	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0.003943	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0	Al2O3(l)**	-381150	2315-5000	3.4620E+01	0.0000E+00	0.0000E+00	0.0000E+00	-1.0320E+04
0.004073	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0.001568	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0.024739	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0.038136	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0.028344	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
0	C2H4(g)	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
0.128142	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0.003968	HNO3(g)	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
0.003968	NOCl(g)	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
0.016344	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0.014172	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0	C12H26(g)	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04
2.16E-05	Fe2O3(s)	-197000	1000-2500	8.0480E+01	-9.1670E-02	6.3250E-05	-1.3760E-08	-2.0440E+04

*Note: Empirical Formula for PBAN is C H1.427 O.095 N.021; This formula and thermal properties are different than PBAN used for T34D Modeling

TABLE F-18. TITAN IV THERMAL PROPERTIES, CASE 2, UPPER CLOUD (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #2 upper cloud

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K) A	B	C	D	E
NH4ClO4(s)	-560.99584						
PBAN	-50.088324						
Al(s)	0						
Fe2O3(s)	-4.2552						
O2(l)	0						
O2(g)	0						
CH1.95	0						
N2O4(l)	-449.8312						
UDMH(l)	456.543						
N2H4(l)	836.5476						
N2(g)	0						
CO2	-955.09806	273-3700	6.4921E-02	1.0257E-04	-3.4578E-08	0.0000E+00	-2.3600E+01
CO	-574.257424	273-3700	1.4087E-01	3.4043E-05	-5.1956E-09	0.0000E+00	-4.3435E+01
H2O	-4044.299454	273-3700	4.8771E-01	2.4239E-04	-3.3867E-08	0.0000E+00	-1.5583E+02
H2	0	273-3700	2.3040E-01	3.7265E-05	-2.7975E-09	0.0000E+00	-7.0297E+01
N2	0	273-3700	9.4216E-01	2.1472E-04	-3.2757E-08	0.0000E+00	-2.9005E+02
HCl	-86.990466	1000-5000	2.1679E-02	1.1269E-05	-3.6828E-09	5.7607E-13	-6.9279E+00
Al2O3(l)	0	2615-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Al2O3(s)	-1631.2365	1000-2315	1.0150E-01	2.1432E-05	-9.1072E-12	-2.0558E-12	-3.1207E+01
NO	33.8688	273-3700	1.0132E-02	3.6973E-06	-1.2074E-09	1.3689E-13	-3.1736E+00
O2	0	273-3700	1.6654E-01	3.7232E-05	-4.4283E-09	0.0000E+00	-5.1234E+01
NH3	-421.02144	273-1500	2.5116E-01	2.3362E-04	9.0230E-08	-6.0941E-11	-8.5920E+01
CH4	-507.045816	1000-5000	8.4641E-02	5.8675E-04	-2.2035E-07	3.8177E-11	-4.9406E+01
C2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO2(g)	1020.01032	273-1500	7.0235E-01	1.7504E-03	-1.0790E-06	2.4091E-10	-2.7807E+02
HNO3(g)	-128.08704	0-1000	3.8081E-02	5.4441E-05	-2.0034E-08	0.0000E+00	-1.3586E+01
NOCl(g)	49.04448	1000-5000	4.2735E-02	1.4301E-05	-5.2735E-09	9.6978E-13	-1.3325E+01
N2H4(g)	366.661296	1000-5000	1.6540E-01	3.0236E-04	-1.0918E-07	1.8289E-11	-6.1780E+01
UDMH(g)	293.43126	0-2000	5.7538E-02	9.2685E-04	-3.0895E-07	0.0000E+00	-5.5568E+01
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C12H26(g)	0	>270	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Fe2O3(s)	-4.2552	1000-2500	1.7384E-03	-1.9801E-06	1.3662E-09	-2.9722E-13	-4.4150E-01

TABLE F-18. TITAN IV THERMAL PROPERTIES, CASE 2, UPPER CLOUD (CONCLUDED).

FIREBALL THERMAL PROPERTIES
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #2 upper cloud

A	B/2	C/3	D/4	E
3.5096E+00	2.2857E-03	-5.8989E-07	5.8940E-11	-1.2339E+03

HEAT OF FORMATION, REACTANTS (calories)	227.920036
HEAT OF FORMATION, PRODUCTS (calories)	-6589.27524
HEAT OF REACTION, (calories)	-6817.19528
FLAME TEMPERATURE (K)	1407

ΔH+AT+B/2T^2+C/3T^3+D/4T^4+E
-0.300602874

TABLE F-19. TITAN IV COEFFICIENTS, CASE 2, LOWER CLOUD.

TITAN IV SOURCE TERM MODEL		
REACTANT AND PRODUCT COMPOSITIONS		
LOWER CLOUD		
test case #2		
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids		
Variable	Description	Value
s	Time of Abort (from launch), seconds	25
A	Altitude at Abort, feet	5000
α	Fraction Total Liquids in Cloud	0
β	Fraction Total Solids in Cloud	0.95
δ	Solid Propellant Reactivity Ratio	1
δ*	Solid Propellant Consumption Ratio	0.772335
γ	Liquid Propellant Reactivity Ratio	0.232
γ*	Liquid Propellant Consumption Ratio	1
ζ	Air Entrainment Ratio, Liquids	0.35
ε	Fraction Excess Hydrazine Monodecomposed	0.7
η	Fraction Excess Hydrazine Vaporized	0.3
ξ	Fraction Excess UDMH Thermally Decomposed	0.5
ι	Fraction Excess UDMH Vaporized	0.5
κ	Fraction Excess Nitrogen Tetroxide Converted to NO2	1
λ	Fraction Excess Nitrogen Tetroxide Thermally Decomposed	0.1
π	Fraction of Solids which Entrain Air	1
ρ	Air Entrainment Ratio, Solids	5.095899
σ	HCl Reactivity	0
SF	Scaling Factor	1.4991E+07

TABLE F-19. TITAN IV COEFFICIENTS, CASE 2, LOWER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
LOWER CLOUD					
test case #2					
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids					
Reactant Composition					
coefficient	value		comments		
a1	0.150779				
a2	0.277125				
a3	0.156796				
a4	0.00041				
a5	0				
a6	0.161355				
a7	0				
a8	0.607001				
a9	0				
a10	0				
a11	0				
a12	0				
a13	0				
a14	0		a14 must be less than or equal to	0.0298312	
a15	0				
a16	0				
a17	0				
a18	0		a18 must be less than or equal to	0.0559672	
a19	0				
a20	0				

TABLE F-19. TITAN IV COEFFICIENTS, CASE 2, LOWER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
LOWER CLOUD					
test case #2					
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids					
Product Composition					
coefficient	value		comment		
b1	0.013193				
b2	0				
b3	0.264029				
b4	0.104867				
b5	0				
b6	0				
b7	0.3191692				
b8	0		b8 must be > or = to 0 (WAS-0.00345, SET TO 0)		
b9	0				
b10	0.078073				
b11	0				
b12	0				
b13	0				
b14	0				
b15	0				
b16	0				
b17	0.607001				
b18	0.149829				
b19	0.07738				
b20	0				
b21	0				
b22	0.00177				
b23	0				
b24	0				
b25	0				
b26	0				
b27	0				
b28	0				
b29	0				
b30	0				
b31	0				
b32	0				
b33	0.00041				

TABLE F-19. TITAN IV COEFFICIENTS, CASE 2, LOWER CLOUD (CONTINUED).

TITAN IV SOURCE TERM MODEL					
REACTANT AND PRODUCT COMPOSITIONS					
LOWER CLOUD					
test case #2					
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids					
SUMMARY					
Consumed	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
NH4ClO4	0.046785	25.78746	181665	117.489	
PBAN	0.085989	47.39622	43376	15.263	
Al	0.048652	26.81645	43385	26.982	
Total	0.181426	100.0001	268427		
REACTANTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
NH4ClO4	0.150779	11.14023	585471	117.489	
PBAN	0.277125	20.47525	139792	15.263	
Al	0.156796	11.58475	139822	26.982	
Fe2O3	0.00041	0.030304	2165	159.692	
O2	0.161355	11.92159	170642	31.999	
N2	0.607001	44.84789	561973	28.013	
N2O4	0	0	0	92.016	
UDMH	0	0	0	60.102	
N2H4	0	0	0	32.045	
Total	1.353465	100.00002	1599865		
PRODUCTS	**g-mole**	**mole %**	**Mass, Lb**	**Mol. Wt.**	
CO2	0.013193	0.81655	19190	44.01	
CO	0.264029	16.34126	244418	28.01	
H2O	0.424036	26.24437	252467	18.015	
H2	0	0	0	2.016	
N2	0.685074	42.40048	634255	28.013	
HCl	0.149829	9.273204	180548	36.461	
Al2O3	0.07738	4.78918	260753	101.961	
NO	0	0	0	30.006	
O2	0.00177	0.109546	1872	31.999	
NH3	0	0	0	17.03	
N2H4(g)	0	0	0	32.045	
CH4	0	0	0	16.04	
UDMH(g)	0	0	0	60.102	
N2O4(g)	0	0	0	92.016	
NO2	0	0	0	46.006	
HNO3	0	0	0	63.013	
NOCl	0	0	0	65.459	
Fe2O3	0.00041	0.025385	2165	159.692	
Total	1.615722	99.99997	1595666		

TABLE F-19. TITAN IV COEFFICIENTS, CASE 2, LOWER CLOUD (CONCLUDED).

TITAN IV SOURCE TERM MODEL			
REACTANT AND PRODUCT COMPOSITIONS			
LOWER CLOUD			
test case #2			
Abort at 5000 ft, Command Destruct, 0.35 moles air/mole liquids			
Adiabatic Flame Temperature, K			3494
Average Molecular Weight (all products), lbs/lb-mole			29.88
Average Molecular Weight (gas products only), lbs/lb-mole			26.22
Fireball Diameter, empirical, feet			780
Fireball Volume, empirical, cubic feet			2.4895E+08
Fireball Diameter, ideal gas, feet			764
Fireball Volume, ideal gas, cubic feet			2.3337E+08
Total Heat Release, calories			-8.082E+11

TABLE F-20. TITAN IV THERMAL PROPERTIES, CASE 2, LOWER CLOUD.

THEORETICAL COMBUSTION PRODUCTS
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #2 lower cloud

MOL. COEFF.	SPECIES	ΔHf CALORIES/MOLE	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/mole-K) A	B	C	D	E
0.150779	NH4ClO4(s)	-70690						
0.277125	PBAN*	-3434						
0.156796	Al(s)	0						
0.00041	Fe2O3(s)	-197000						
0	O2(l)	-3124						
0.161355	O2(g)	0						
0	CH1.95	-6220						
0	N2O4(l)	-4676						
0	UDMH(l)	12339						
0	N2H4(l)	12054						
0.607001	N2(g)	0						
0.013193	CO2	-94052	273-3700	6.3930E+00	1.0100E-02	-3.4050E-06	0.0000E+00	-2.3240E+03
0.264029	CO	-26416	273-3700	6.4800E+00	1.5660E-03	-2.3900E-07	0.0000E+00	-1.9980E+03
0.424036	H2O	-57798	273-3700	6.9700E+00	3.4640E-03	-4.8400E-07	0.0000E+00	-2.2270E+03
0	H2	0	273-3700	6.4240E+00	1.0390E-03	-7.8000E-08	0.0000E+00	-1.9600E+03
0.685074	N2	0	273-3700	6.5290E+00	1.4880E-03	-2.2700E-07	0.0000E+00	-2.0100E+03
0.149829	HCl	-22062	1000-5000	5.4980E+00	2.8580E-03	-9.3400E-07	1.4610E-10	-1.7570E+03
0.07738	Al2O3(l)**	-381150	2315-5000	3.4620E+01	0.0000E+00	0.0000E+00	0.0000E+00	-1.0320E+04
0	Al2O3(s)	-400500	1000-2315	2.4919E+01	5.2620E-03	-2.2360E-09	-5.0475E-10	-7.6620E+03
0	NO	21600	273-3700	6.4620E+00	2.3580E-03	-7.7000E-07	8.7300E-11	-2.0240E+03
0.00177	O2	0	273-3700	6.7320E+00	1.5050E-03	-1.7900E-07	0.0000E+00	-2.0710E+03
0	NH3	-11040	273-1500	6.5860E+00	6.1260E-03	2.3660E-06	-1.5980E-09	-2.2530E+03
0	CH4	-17889	1000-5000	2.9862E+00	2.0701E-02	-7.7740E-06	1.3469E-09	-1.7431E+03
0	C2H4(g)	12496	1000-5000	6.8662E+00	2.2837E-02	-8.6740E-06	1.5134E-09	-2.9866E+03
0	NO2(g)	7960	273-1500	5.4810E+00	1.3660E-02	-8.4200E-06	1.8800E-09	-2.1700E+03
0	HNO3(g)	-32280	0-1000	9.5970E+00	1.3720E-02	-5.0490E-06	0.0000E+00	-3.4240E+03
0	NOCl(g)	12360	1000-5000	1.0770E+01	3.6040E-03	-1.3290E-06	2.4440E-10	-3.3580E+03
0	N2H4(g)	22434	1000-5000	1.0120E+01	1.8500E-02	-6.6800E-06	1.1190E-09	-3.7800E+03
0	UDMH(g)	20705	0-2000	4.0600E+00	6.5400E-02	-2.1800E-05	0.0000E+00	-3.9210E+03
0	N2O4(g)	2114	273-1500	7.9450E+00	4.4600E-02	-2.7100E-05	0.0000E+00	-4.1090E-03
0	C12H26(g)	-69526	>270	5.1624E+00	2.5650E-01	-1.3674E-04	2.8230E-08	-1.1777E+04
0.00041	Fe2O3(s)	-197000	1000-2500	8.0480E+01	-9.1670E-02	6.3250E-05	-1.3760E-08	-2.0440E+04

*Note: Empirical Formula for PBAN is C H1.427 O.095 N.021; This formula and thermal properties are different than PBAN used for T34D Modeling

TABLE F-20. TITAN IV THERMAL PROPERTIES, CASE 2, LOWER CLOUD (CONTINUED).

THEORETICAL COMBUSTION PRODUCTS (SCALED BY MOLAR QTY)
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #2 lower cloud

SPECIES	ΔHf CALORIES	TEMP RANGE (KELVIN)	Cp, HEAT CAPACITY, (calories/K)				
			A	B	C	D	E
NH4ClO4(s)	-10658.56751						
PBAN	-951.64725						
Al(s)	0						
Fe2O3(s)	-80.77						
O2(l)	0						
O2(g)	0						
CH1.95	0						
N2O4(l)	0						
UDMH(l)	0						
N2H4(l)	0						
N2(g)	0						
CO2	-1240.828036	273-3700	8.4343E-02	1.3325E-04	-4.4922E-08	0.0000E+00	-3.0661E+01
CO	-6974.590064	273-3700	1.7109E+00	4.1347E-04	-6.3103E-08	0.0000E+00	-5.2753E+02
H2O	-24508.43273	273-3700	2.9555E+00	1.4689E-03	-2.0523E-07	0.0000E+00	-9.4433E+02
H2	0	273-3700	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2	0	273-3700	4.4728E+00	1.0194E-03	-1.5551E-07	0.0000E+00	-1.3770E+03
HCl	-3305.527398	1000-5000	8.2376E-01	4.2821E-04	-1.3994E-07	2.1890E-11	-2.6325E+02
Al2O3(l)	-29493.387	2615-5000	2.6789E+00	0.0000E+00	0.0000E+00	0.0000E+00	-7.9856E+02
Al2O3(s)	0	1000-2315	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO	0	273-3700	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
O2	0	273-3700	1.1916E-02	2.6639E-06	-3.1683E-10	0.0000E+00	-3.6657E+00
NH3	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
CH4	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NO2(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
HNO3(g)	0	0-1000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
NOCl(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2H4(g)	0	1000-5000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
UDMH(g)	0	0-2000	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
N2O4(g)	0	273-1500	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
C12H26(g)	0	>270	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Fe2O3(s)	-80.77	1000-2500	3.2997E-02	-3.7585E-05	2.5933E-08	-5.6416E-12	-8.3804E+00

TABLE F-20. TITAN IV THERMAL PROPERTIES, CASE 2, LOWER CLOUD (CONCLUDED).

FIREBALL THERMAL PROPERTIES
LAUNCH VEHICLE ABORT SOURCE STRENGTH MODEL
CONDITION/MATERIAL TESTED: TITAN IV MODEL test case #2 lower cloud

A	B/2	C/3	D/4	E
1.2771E+01	1.7141E-03	-1.9436E-07	4.0621E-12	-3.9534E+03

HEAT OF FORMATION, REACTANTS (calories)	-11690.9848
HEAT OF FORMATION, PRODUCTS (calories)	-65603.5352
HEAT OF REACTION, (calories)	-53912.5505
FLAME TEMPERATURE (K)	3494

ΔH+AT+B/2T^2+C/3T^3+D/4T^4+E
-2.413771089

TABLE F-21. TITAN IV CSD SOLIDS, COMPOSITION AND THERMAL PROPERTIES.

SOLID FIREBALL CHARACTERISTICS

INITIAL CONDITIONS:

brsa= 0.002794
nsia= 1
mss= 29785743
awt= 0.8

msia= 29785743
gsia= 664165.19
burn time= 286.33

SOLIDS HEAT OF REACTION= -5.279E+10 (cal.)
TOTAL MOLES PRODUCT= 1550982.8
ABAR= 8.0892601
BBAR= 0.0020382
CBAR= -3.663E-07
DBAR= 1.602E-11
EBAR= -2497.9012

Solids Cloud Effective Fireball Diameter (m)= 95.09
Solids Cloud Effective Fireball Volume (m^3)= 450131.67

ADIABATIC FLAME TEMP.
SOLIDS (°C)= 3262
SOLIDS (K)= 3535

SOLID CLOUD CHEMICAL COMPOSITION

REACTANT SPECIES	H	V	T	B	M	E	C	S	X	SUM MOLES	MW	SUM GRAMS REACT.
N2O4 (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	92.01	0.0000E+00
UDMH (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	60.099	0.0000E+00
Hydrazine (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	32.045	0.0000E+00
LOX	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	32	0.0000E+00
RP-1 (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.98	0.0000E+00
Iron Oxide (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	464.9	0.0	464.9	159.69	7.4242E+04
Aluminum (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	177929.9	0.0	177929.9	26.98	4.8005E+06
Ammonium Perchlorate	0.0	0.0	0.0	0.0	0.0	0.0	0.0	171155.4	0.0	171155.4	117.49	2.0109E+07
(HTPB) (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.65	0.0000E+00
(PBAN) (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	314615.0	0.0	314615.0	15.263	4.8021E+06
Nitrogen	0.0	0.0	0.0	0.0	0.0	407953.1	0.0	0.0	0.0	407953.1	28.013	1.1428E+07
Oxygen	0.0	0.0	0.0	0.0	0.0	108443.2	0.0	0.0	0.0	108443.2	31.999	3.4701E+06
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00

TABLE F-21. TITAN IV CSD SOLIDS, COMPOSITION AND THERMAL PROPERTIES (CONTINUED).

PRODUCT SPECIES	H	V	T	B	M	E	C	S	X	SUM MOLES	MW	PROD.SUM GRAMS
Nitrogen Tetroxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	92.01	0
UDMH (g)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	60.099	0
Hydrazine (g)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	32.045	0
RP-1 (g)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	170.34	0
Carbon Dioxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	14976.1	0.0	14976.1	44.01	659097.9286
Carbon Monoxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	299710.2	0.0	299710.2	28.01	8394881.729
Methane	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	16.043	0
Water	0.0	0.0	0.0	0.0	0.0	216886.5	0.0	119038.6	0.0	335925.0	18.015	6051689.537
Ammonia	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.03	0
Nitrogen Dioxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	46.006	0
Nitric Oxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	30.006	0
Nitric Acid	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	63.013	0
Nitrogen	0.0	0.0	0.0	0.0	0.0	407953.1	0.0	88624.2	0.0	496577.4	28.013	13910622.35
Oxygen	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	31.999	0
Oxygen Radical	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	16	0
Hydrogen	0.0	0.0	0.0	0.0	0.0	0.0	0.0	145415.2	0.0	145415.2	2.016	293157.0538
Hydrogen Ion	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.008	0
Hydrochloric Acid	0.0	0.0	0.0	0.0	0.0	0.0	0.0	170077.1	0.0	170077.1	36.46	6201010.679
Aluminum Oxide (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	101.96	0
Hydroxide Ion	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.007	0
Aluminum Oxide (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	87836.9	0.0	87836.9	101.96	8955853.889
Aluminum Chloride	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	62.43	0
Chlorine Ion	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	35.45	0
Nitrosyl Chloride NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	65.46	0
Ethylene C2H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	28.05	0
Iron Oxide (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	464.9	0.0	464.9	159.69	74242.37689
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
								SUM MOLES PRODUCTS= 1.5510E+06				44540555.54

SUM GRAMS REACTANTS= 44683983.2
SUM GRAMS PRODUCTS= 44540555.5
MASSBALANCE= 1.43E+05
% DELTA= 0.320982294

TABLE F-22. DELTA II GEMs SOLIDS, COMPOSITION AND THERMAL PROPERTIES.

SOLID FIREBALL CHARACTERISTICS

INITIAL CONDITIONS:

brsa= 0.00254
nsla= 1
mss= 11702622
awt= 0.4
nspm= 1
msla= 11702622
gsla= 249050.25
burn time= 157.48031

SOLIDS HEAT OF REACTION= -2.23E+10 (cal.)
TOTAL MOLES PRODUCT= 578603.25
ABAR= 8.4320725
BBAR= 0.0020836
CBAR= -3.772E-07
DBAR= 1.696E-11
EBAR= -2601.9827

Solids Cloud Effective Fireball Diameter (m)= 70.14961058
Solids Cloud Effective Fireball Volume (m^3)= 180750.16

ADIABATIC FLAME TEMP.
SOLIDS (°C)= 3532
SOLIDS (K)= 3805

SOLID CLOUD CHEMICAL COMPOSITION

REACTANT SPECIES	H	V	T	B	M	E	C	S	X	SUM MOLES	MW	SUM GRAMS REACT.
N2O4 (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	92.01	0.0000E+00
UDMH (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	60.099	0.0000E+00
Hydrazine (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	32.045	0.0000E+00
LOX	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	32	0.0000E+00
RP-1 (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.98	0.0000E+00
Iron Oxide (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	159.69	0.0000E+00
Aluminum (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	83108.1	0.0	83108.1	26.98	2.2423E+06
Ammonium Perchlorate	0.0	0.0	0.0	0.0	0.0	0.0	0.0	69377.9	0.0	69377.9	117.49	8.1512E+06
(HTPB) (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	96564.3	0.0	96564.3	13.65	1.3181E+06
(PBAN) (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.263	0.0000E+00
Nitrogen	0.0	0.0	0.0	0.0	0.0	160282.1	0.0	0.0	0.0	160282.1	28.013	4.4900E+06
Oxygen	0.0	0.0	0.0	0.0	0.0	42606.6	0.0	0.0	0.0	42606.6	31.999	1.3634E+06
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0.0000E+00

TABLE F-22. DELTA II GEMs SOLIDS, COMPOSITION AND THERMAL PROPERTIES (CONCLUDED).

PRODUCT SPECIES	H	V	T	B	M	E	C	S	X	SUM MOLES	MW	PROD.SUM GRAMS
Nitrogen Tetroxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	92.01	0
UDMH (g)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	60.099	0
Hydrazine (g)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	32.045	0
RP-1 (g)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	170.34	0
Carbon Dioxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5605.7	0.0	5605.7	44.01	246708.4633
Carbon Monoxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	90010.9	0.0	90010.9	28.01	2521205.938
Methane	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	16.043	0
Water	0.0	0.0	0.0	0.0	0.0	85213.3	0.0	54135.6	0.0	139348.9	18.015	2510369.774
Ammonia	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.03	0
Nitrogen Dioxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	46.006	0
Nitric Oxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	30.006	0
Nitric Acid	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	63.013	0
Nitrogen	0.0	0.0	0.0	0.0	0.0	160282.1	0.0	34536.3	0.0	194818.4	28.013	5457448.665
Oxygen	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	31.999	0
Oxygen Radical	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	16	0
Hydrogen	0.0	0.0	0.0	0.0	0.0	0.0	0.0	41852.4	0.0	41852.4	2.016	84374.45102
Hydrogen Ion	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.008	0
Hydrochloric Acid	0.0	0.0	0.0	0.0	0.0	0.0	0.0	67150.9	0.0	67150.9	36.46	2448321.651
Aluminum Oxide (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	101.96	0
Hydroxide Ion	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	17.007	0
Aluminum Oxide (l)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	39816.0	0.0	39816.0	101.96	4059638.574
Aluminum Chloride	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	62.43	0
Chlorine Ion	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	35.45	0
Nitrosyl Chloride NO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	65.46	0
Ethylene C2H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	28.05	0
Iron Oxide (s)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	159.69	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0
Not Used	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	0

SUM MOLES PRODUCTS= 5.7860E+05

17328067.52

SUM GRAMS REACTANTS= 17564922.4
SUM GRAMS PRODUCTS= 17328067.5
MASSBALANCE= 2.37E+05
% DELTA= 1.348453838